

SAFETY DATA SHEET

Version 6.6
Revision Date 09/06/2024
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SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifiers**

Product name : Methyl 4-hydroxybenzoate

Product Number : H3647
Brand : Sigma
CAS-No. : 99-76-3

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

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone : +1 314 771-5765
Fax : +1 800 325-5052

1.4 Emergency telephone

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2: Hazards identification**2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Short-term (acute) aquatic hazard (Category 3), H402
Long-term (chronic) aquatic hazard (Category 2), H411

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

2.2 GHS Label elements, including precautionary statements

Pictogram



Signal Word

none

Hazard Statements

H402

Harmful to aquatic life.

H411

Toxic to aquatic life with long lasting effects.

Precautionary Statements

P273

Avoid release to the environment.

P391

Collect spillage.

P501

Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

SECTION 3: Composition/information on ingredients

3.1 Substances

Synonyms : Methyl paraben
p-Hydroxybenzoic acid methyl ester

Formula : C₈H₈O₃

Molecular weight : 152.15 g/mol

CAS-No. : 99-76-3

EC-No. : 202-785-7

Component	Classification	Concentration
methyl 4-hydroxybenzoate		
	Aquatic Acute 3; Aquatic Chronic 2; H402, H411	<= 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

If inhaled

After inhalation: fresh air.

In case of skin contact

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

In case of eye contact

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

If swallowed

After swallowing: make victim drink water (two glasses at most). Consult doctor if feeling unwell.

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

In the event of fire, wear self-contained breathing apparatus.

5.4 Further information

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. 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

Tightly closed. Dry.

Storage class

Storage class (TRGS 510): 11: Combustible Solids

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

Appropriate engineering controls

Change contaminated clothing. Wash hands after working with substance.

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: 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 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: 0.11 mm

Break through time: 480 min
Material tested: KCL 741 Dermatril® L

Respiratory protection

Recommended Filter type: Filter type P1

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.

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.

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: solid Color: white
b) Odor	odorless
c) Odor Threshold	Not applicable
d) pH	5.72 at 1.88 g/l at 20 °C (68 °F)
e) Melting point/freezing point	Melting point/ range: 125 - 128 °C (257 - 262 °F) - lit.
f) Initial boiling point and boiling range	Decomposes below the boiling point.
g) Flash point	168 °C (334 °F)
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	< 1 hPa at 20 °C (68 °F)
l) Vapor density	5.23 - (Air = 1.0)
m) Density	1.38 g/cm ³ at 20 °C (68 °F) - OECD Test Guideline 109
Relative density	No data available
n) Water solubility	1.88 g/l at 20 °C (68 °F) - OECD Test Guideline 105
o) Partition coefficient: n-octanol/water	Pow: 95.5; log Pow: 1.98 at 22 °C (72 °F) - Bioaccumulation is not expected.

- | | |
|------------------------------|---|
| p) Autoignition temperature | > 403 °C (> 757 °F) - Relative self-ignition temperature for solids |
| q) Decomposition temperature | 270 - 280 °C (518 - 536 °F) - |
| r) Viscosity | No data available |
| s) Explosive properties | No data available |
| t) Oxidizing properties | none |

9.2 Other safety information

Relative vapor density	5.23 - (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.
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

Violent reactions possible with:
Bases
Strong oxidizing agents

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 - > 5,000 mg/kg
(OECD Test Guideline 401)
Inhalation: No data available
Dermal: No data available

Sigma - H3647

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Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation

Remarks: (External MSDS)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: slight irritation

Remarks: (ECHA)

Respiratory or skin sensitization

Maurer optimisation test - Guinea pig

Result: negative

(OECD Test Guideline 406)

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: In vitro mammalian cell gene mutation test

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 476

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: negative

Test Type: dominant lethal test

Species: Rat

Application Route: Oral

Method: OECD Test Guideline 478

Result: negative

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.

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.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

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

RTECS: DH2450000

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated., Respiratory disorders, Discomfort, giddiness, Nausea, Vomiting

SECTION 12: Ecological information**12.1 Toxicity**

Toxicity to fish	semi-static test LC50 - <i>Oryzias latipes</i> (Orange-red killifish) - 59.5 mg/l - 96 h (OECD Test Guideline 203) Remarks: (ECHA)
	NOEC - <i>Danio rerio</i> (zebra fish) - 0.024 mg/l Remarks: (ECHA)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - <i>Daphnia magna</i> (Water flea) - 11.2 mg/l - 48 h (ISO 6341) Remarks: (ECHA)
	semi-static test NOEC - <i>Daphnia magna</i> (Water flea) - 0.20 mg/l - 21 d Remarks: (ECHA)
Toxicity to algae	static test ErC50 - <i>Pseudokirchneriella subcapitata</i> (algae) - 91 mg/l - 72 h (ISO 8692) Remarks: (ECHA)
Toxicity to bacteria	EC0 - <i>Pseudomonas fluorescens</i> - 500 mg/l Remarks: (External MSDS)

12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 28 d Result: 89 % - Readily biodegradable. (OECD Test Guideline 301B)
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12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Endocrine disrupting properties

No data available

12.7 Other adverse effects

No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

SECTION 14: Transport information

DOT (US)

Not dangerous goods

IMDG

UN number: 3077

Class: 9

Packing group: III

EMS-

No: F-A, S-F

Proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (methyl 4-hydroxybenzoate)

Marine pollutant : yes

Marine pollutant : no

IATA

UN number: 3077 Class: 9

Packing group: III

Proper shipping name: Environmentally hazardous substance, solid, n.o.s. (methyl 4-hydroxybenzoate)

Further information

EHS-Mark required (ADR 2.2.9.1.10, IMDG code 2.10.3) for single packagings and combination packagings containing inner packagings with Dangerous Goods > 5L for liquids or > 5kg for solids. Packages smaller than or equal to 5 kg / L , not dangerous goods of Class 9

SECTION 15: Regulatory information

CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

This material does not contain any components with a section 302 EHS TPQ.

SARA 311/312 Hazards : No SARA Hazards

SARA 313 : This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

US State Regulations

Massachusetts Right To Know

No components are subject to the Massachusetts Right to Know Act.

Maine Chemicals of High Concern

methyl 4-hydroxybenzoate 99-76-3

Vermont Chemicals of High Concern

methyl 4-hydroxybenzoate 99-76-3

Washington Chemicals of High Concern

methyl 4-hydroxybenzoate 99-76-3

The ingredients of this product are reported in the following inventories:

TSCA : All substances listed as active on the TSCA inventory

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16: Other information

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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