

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 23.03.2017

Version 12.2

SECTION 1. Identification of the substance/mixture and of the company/undertaking**1.1 Product identifier**

Catalogue No. 818701

Product name Benzyl benzoate for synthesis

REACH Registration Number A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

CAS-No. 120-51-4

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.

SECTION 2. Hazards identification**2.1 Classification of the substance or mixture****Classification (REGULATION (EC) No 1272/2008)**

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 818701
Product name Benzyl benzoate for synthesis

Acute toxicity, Category 4, Oral, H302

Acute aquatic toxicity, Category 1, H400

Chronic aquatic toxicity, Category 2, H411

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

2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

Hazard pictograms



Signal word

Warning

Hazard statements

H302 Harmful if swallowed.

H410 Very toxic to aquatic life with long lasting effects.

Precautionary statements

Prevention

P273 Avoid release to the environment.

Reduced labelling (≤ 125 ml)

Hazard pictograms



Signal word

Warning

Index-No. 607-085-00-9

2.3 Other hazards

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 818701
Product name Benzyl benzoate for synthesis

None known.

SECTION 3. Composition/information on ingredients

3.1 Substance

Formula	$C_6H_5COOCH_2C_6H_5$	$C_{14}H_{12}O_2$ (Hill)
Index-No.	607-085-00-9	
EC-No.	204-402-9	
Molar mass	212,24 g/mol	

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

Chemical name (Concentration)

CAS-No.	Registration number	Classification
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Benzyl benzoate ($\leq 100\%$)

120-51-4 *)

Acute toxicity, Category 4, H302

Acute aquatic toxicity, Category 1, H400

Chronic aquatic toxicity, Category 2, H411

*) A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

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.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 818701
Product name Benzyl benzoate for synthesis

After eye contact: rinse out with plenty of water. 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, agitation, spasms, Diarrhoea, Nausea, Vomiting, cardiovascular disorders, ataxia (impaired locomotor coordination)

4.3 Indication of any immediate medical attention and special treatment needed

No information 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

Combustible.

Vapours 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

Special protective equipment for firefighters

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

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

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 818701
Product name Benzyl benzoate for synthesis

Advice for non-emergency personnel: Do not breathe vapours, aerosols. 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.

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

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

Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed.

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.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 818701
Product name Benzyl benzoate for synthesis

SECTION 8. Exposure controls/personal protection

8.1 Control parameters

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

Hand protection

full contact:

Glove material:	butyl-rubber
Glove thickness:	0,7 mm
Break through time:	> 480 min

splash contact:

Glove material:	Nitrile rubber
Glove thickness:	0,40 mm
Break through time:	> 30 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 898 Butoject® (full contact), KCL 730 Camatril® -Velours (splash contact).

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 818701
Product name Benzyl benzoate for synthesis

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 vapours/aerosols are generated.

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.

Environmental exposure controls

Do not let product enter drains.

SECTION 9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

Form	liquid
Colour	colourless
Odour	weakly aromatic
Odour Threshold	No information available.
pH	No information available.
Melting point	21 °C
Boiling point/boiling range	324 °C at 1.013 hPa

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 818701
Product name Benzyl benzoate for synthesis

Flash point	158 °C Method: c.c.
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	< 0,1 hPa at 25 °C
Relative vapour density	7,31
Density	1,12 g/cm ³ at 20 °C
Relative density	No information available.
Water solubility	0,0153 g/l at 20 °C
Partition coefficient: n-octanol/water	log Pow: 3,97 (25 °C) (experimental) (Lit.) Bioaccumulation is not expected.
Auto-ignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	10,9 mPa.s at 25 °C

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	818701
Product name	Benzyl benzoate for synthesis

Explosive properties Not classified as explosive.

Oxidizing properties none

9.2 Other data

Ignition temperature 480 °C

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

10.4 Conditions to avoid

Strong heating.

10.5 Incompatible materials

various plastics, Light metals, metal alloys

10.6 Hazardous decomposition products

no information available

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 818701
Product name Benzyl benzoate for synthesis

SECTION 11. Toxicological information

11.1 Information on toxicological effects

Acute oral toxicity

LD50 Rat: 1.904 mg/kg

(RTECS)

Symptoms: Nausea, Vomiting, Diarrhoea

Acute inhalation toxicity

Symptoms: Irritation symptoms in the respiratory tract.

Acute dermal toxicity

LD50 Rabbit: 4.000 mg/kg

(RTECS)

Skin irritation

Rabbit

Result: No skin irritation

OECD Test Guideline 404

Eye irritation

Rabbit

Result: No eye irritation

OECD Test Guideline 405

Sensitisation

Patch test: human

Result: negative

(IUCLID)

Sensitisation test: Guinea pig

Result: negative

(IUCLID)

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 818701
Product name Benzyl benzoate for synthesis

Sensitisation test: Mouse
Result: negative
Method: OECD Test Guideline 429

Germ cell mutagenicity

Genotoxicity in vitro

Ames test

Result: negative

(IUCLID)

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

Systemic effects:

cardiovascular disorders, agitation, spasms, ataxia (impaired locomotor coordination)

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

12.1 Toxicity

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 818701
Product name Benzyl benzoate for synthesis

Toxicity to fish

semi-static test LC50 Danio rerio (zebra fish): 0,29 mg/l; 96 h

Analytical monitoring: yes

Directive 67/548/EEC, Annex V, C.1.

Toxicity to daphnia and other aquatic invertebrates

static test EC50 Daphnia magna (Water flea): 3,09 mg/l; 48 h

Analytical monitoring: yes

OECD Test Guideline 202

Toxicity to algae

static test ErC50 Pseudokirchneriella subcapitata (green algae): 0,475 mg/l; 72 h

Analytical monitoring: yes

OECD Test Guideline 201

Toxicity to bacteria

static test EC50 activated sludge: > 10.000 mg/l; 3 h

OECD Test Guideline 209

12.2 Persistence and degradability

Biodegradability

94 %; 28 d; aerobic

C.4-D of the COUNCIL REGULATION (EC) No 440/2008

Readily biodegradable

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 3,97 (25 °C)

(experimental)

(Lit.) Bioaccumulation is not expected.

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.

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 818701
Product name Benzyl benzoate for synthesis

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 3082
14.2 Proper shipping name ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID,
N.O.S. (BENZYL BENZOATE)
14.3 Class 9
14.4 Packing group III
14.5 Environmentally hazardous yes
14.6 Special precautions for user yes
Tunnel restriction code E

Packages smaller than or equal to 5 kg / L , not dangerous goods of Class 9

Inland waterway transport (ADN)

Not relevant

Air transport (IATA)

14.1 UN number UN 3082
14.2 Proper shipping name ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID,
N.O.S. (BENZYL BENZOATE)
14.3 Class 9
14.4 Packing group III
14.5 Environmentally hazardous yes

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 818701
Product name Benzyl benzoate for synthesis

14.6 Special precautions for user no

Packages smaller than or equal to 5 kg / L , not dangerous goods of Class 9

Sea transport (IMDG)

14.1 UN number UN 3082

14.2 Proper shipping name ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (BENZYL BENZOATE)

14.3 Class 9

14.4 Packing group III

14.5 Environmentally hazardous yes

14.6 Special precautions for user yes

EmS F-A S-F

Packages smaller than or equal to 5 kg / L , not dangerous goods of Class 9

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 ENVIRONMENTAL HAZARDS

E1

Quantity 1: 100 t

Quantity 2: 200 t

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.

Regulation (EC) No 1005/2009 on substances that deplete the ozone layer not regulated

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 818701
Product name Benzyl benzoate for synthesis

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 ≥ 0.1 % (w/w).

National legislation

Storage class 10 - 13

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.

H302 Harmful if swallowed.
H400 Very toxic to aquatic life.
H411 Toxic to aquatic life with long lasting effects.

Training advice

Provide adequate information, instruction and training for operators.

Labelling

Hazard pictograms



SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	818701
Product name	Benzyl benzoate for synthesis

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H400 Very toxic to aquatic life.

H411 Toxic to aquatic life with long lasting effects.

Precautionary statements

Prevention

P273 Avoid release to the environment.

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.