

# Voluntary safety information following the Safety Data Sheet format according to Regulation (EC) No. 1907/2006 (REACH)



## Benzoic acid ethyl ester $\geq$ 99%, for synthesis

article number: **0880**  
Version: **3.2 en**  
Replaces version of: 04.03.2024  
Version: (3)

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

### 1.1 Product identifier

Identification of the substance	<b>Benzoic acid ethyl ester <math>\geq</math> 99%, for synthesis</b>
Article number	0880
Registration number (REACH)	It is not required to list the identified uses because the substance is not subject to registration according to REACH (< 1 t/a).
EC number	202-284-3
CAS number	93-89-0

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

Relevant identified uses:	Laboratory chemical Laboratory and analytical use
Uses advised against:	Do not use for private purposes (household). Food, drink and animal feedingstuffs.

### 1.3 Details of the supplier of the safety data sheet

Carl Roth GmbH + Co. KG  
Schoemperlenstr. 3-5  
D-76185 Karlsruhe  
Germany

**Telephone:** +49 (0) 721 - 56 06 0

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**e-mail:** [sicherheit@carlroth.de](mailto:sicherheit@carlroth.de)

**Website:** [www.carlroth.de](http://www.carlroth.de)

Competent person responsible for the safety data sheet: Department Health, Safety and Environment

**e-mail (competent person):** [sicherheit@carlroth.de](mailto:sicherheit@carlroth.de)

### 1.4 Emergency telephone number

## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

#### Classification according to Regulation (EC) No 1272/2008 (CLP)

This substance does not meet the criteria for classification in accordance with Regulation No 1272/2008/EC.

### 2.2 Label elements

#### Labelling according to Regulation (EC) No 1272/2008 (CLP)

not required

### 2.3 Other hazards

This material is combustible, but will not ignite readily.

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**Results of PBT and vPvB assessment**

According to the results of its assessment, this substance is not a PBT or a vPvB.

**Endocrine disrupting properties**

Does not contain an endocrine disruptor (ED) at a concentration of  $\geq$  0,1%.

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Name of substance	Benzoic acid ethyl ester
Molecular formula	$C_9H_{10}O_2$
Molar mass	150,2 $g/mol$
CAS No	93-89-0
EC No	202-284-3

## SECTION 4: First aid measures

### 4.1 Description of first aid measures



**General notes**

Take off contaminated clothing.

**Following inhalation**

Provide fresh air.

**Following skin contact**

Rinse skin with water/shower.

**Following eye contact**

Rinse cautiously with water for several minutes.

**Following ingestion**

Rinse mouth. Call a doctor if you feel unwell.

### 4.2 Most important symptoms and effects, both acute and delayed

Causes slight to moderate irritation, Cough, Breathing difficulties, May cause drowsiness or dizziness

### 4.3 Indication of any immediate medical attention and special treatment needed

none

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## SECTION 5: Firefighting measures

### 5.1 Extinguishing media



#### Suitable extinguishing media

co-ordinate firefighting measures to the fire surroundings!  
water spray, dry extinguishing powder, BC-powder, carbon dioxide (CO<sub>2</sub>)

#### Unsuitable extinguishing media

water jet

### 5.2 Special hazards arising from the substance or mixture

Combustible. Vapours are heavier than air, spread along floors and form explosive mixtures with air.

#### Hazardous combustion products

In case of fire may be liberated: Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>)

### 5.3 Advice for firefighters

In case of fire and/or explosion do not breathe fumes. Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus.

## SECTION 6: Accidental release measures

### 6.1 Personal precautions, protective equipment and emergency procedures



#### For non-emergency personnel

No special measures are necessary.

### 6.2 Environmental precautions

Keep away from drains, surface and ground water. Retain contaminated washing water and dispose of it.

### 6.3 Methods and material for containment and cleaning up

#### Advice on how to contain a spill

Covering of drains.

#### Other information relating to spills and releases

Place in appropriate containers for disposal. Ventilate affected area.

### 6.4 Reference to other sections

Hazardous combustion products: see section 5. Personal protective equipment: see section 8. Incompatible materials: see section 10. Disposal considerations: see section 13.

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## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

Provision of sufficient ventilation.

**Measures to prevent fire as well as aerosol and dust generation**



Keep away from sources of ignition - No smoking.

**Advice on general occupational hygiene**

Keep away from food, drink and animal feedingstuffs.

### 7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed.

**Incompatible substances or mixtures**

Observe hints for combined storage.

**Consideration of other advice:**

**Specific designs for storage rooms or vessels**

Recommended storage temperature: 15 – 25 °C

### 7.3 Specific end use(s)

No information available.

## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

**National limit values**

**Occupational exposure limit values (Workplace Exposure Limits)**

This information is not available.

**Human health values**

Relevant DNELs and other threshold levels				
Endpoint	Threshold level	Protection goal, route of exposure	Used in	Exposure time
DNEL	17,5 mg/m <sup>3</sup>	human, inhalatory	worker (industry)	chronic - systemic effects
DNEL	5 mg/kg bw/day	human, dermal	worker (industry)	chronic - systemic effects

**Environmental values**

Relevant PNECs and other threshold levels				
End-point	Threshold level	Organism	Environmental compartment	Exposure time
PNEC	0,007 mg/l	aquatic organisms	freshwater	short-term (single instance)
PNEC	0,001 mg/l	aquatic organisms	marine water	short-term (single instance)

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Relevant PNECs and other threshold levels				
End-point	Threshold level	Organism	Environmental compartment	Exposure time
PNEC	0,31 mg/l	aquatic organisms	sewage treatment plant (STP)	short-term (single instance)
PNEC	0,18 mg/kg	aquatic organisms	freshwater sediment	short-term (single instance)
PNEC	0,018 mg/kg	aquatic organisms	marine sediment	short-term (single instance)
PNEC	0,032 mg/kg	terrestrial organisms	soil	short-term (single instance)

## 8.2 Exposure controls

### Individual protection measures (personal protective equipment)

#### Eye/face protection



Use safety goggle with side protection.

#### Skin protection



- **hand protection**

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374.

- **type of material**

Butyl caoutchouc (butyl rubber)

- **material thickness**

0,5 mm

- **breakthrough times of the glove material**

>480 minutes (permeation: level 6)

- **other protection measures**

Take recovery periods for skin regeneration. Preventive skin protection (barrier creams/ointments) is recommended.

#### Respiratory protection



Respiratory protection necessary at: Aerosol or mist formation. Type: A (against organic gases and vapours with a boiling point of  $> 65$  °C, colour code: Brown).

#### Environmental exposure controls

Keep away from drains, surface and ground water.

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## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

Physical state	liquid
Colour	colourless
Odour	mild sweet - fruity
Odour threshold	0,6 ppm
Melting point/freezing point	-35 °C
Boiling point or initial boiling point and boiling range	212 – 215 °C
Flammability	this material is combustible, but will not ignite readily
Lower and upper explosion limit	1 vol% (LEL)
Flash point	88 °C (c.c.)
Auto-ignition temperature	460 °C at 1.004 hPa (ECHA)
Decomposition temperature	not relevant
pH (value)	not determined
Kinematic viscosity	not determined
<u>Solubility(ies)</u>	
Water solubility	0,72 g/l at 25 °C
<u>Partition coefficient</u>	
Partition coefficient n-octanol/water (log value):	2,59 (22,8 °C) (ECHA)
<u>Vapour pressure</u>	
	0,24 hPa at 20 °C 1,3 hPa at 44 °C
<u>Density and/or relative density</u>	
Density	1,05 g/cm <sup>3</sup> at 20 °C
Relative vapour density	5,19 (air = 1)
Particle characteristics	not relevant (liquid)
<u>Other safety parameters</u>	
Oxidising properties	none

### 9.2 Other information

Information with regard to physical hazard classes:	hazard classes acc. to GHS (physical hazards): not relevant
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Other safety characteristics:

Temperature class (EU, acc. to ATEX)

T1  
Maximum permissible surface temperature on the equipment: 450°C

## SECTION 10: Stability and reactivity

### 10.1 Reactivity

This material is not reactive under normal ambient conditions.

#### If heated

Vapours may form explosive mixtures with air.

### 10.2 Chemical stability

The material is stable under normal ambient and anticipated storage and handling conditions of temperature and pressure.

### 10.3 Possibility of hazardous reactions

**Violent reaction with:** strong oxidiser, Bases

### 10.4 Conditions to avoid

Keep away from heat.

### 10.5 Incompatible materials

There is no additional information.

### 10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

## SECTION 11: Toxicological information

### 11.1 Information on hazard classes as defined in Regulation (EC) No 1272/2008

#### Classification according to GHS (1272/2008/EC, CLP)

This substance does not meet the criteria for classification in accordance with Regulation No 1272/2008/EC.

#### Acute toxicity

Shall not be classified as acutely toxic.

Acute toxicity					
Exposure route	Endpoint	Value	Species	Method	Source
oral	LD50	2.100 mg/kg	rat		TOXNET

#### Skin corrosion/irritation

Shall not be classified as corrosive/irritant to skin.

#### Serious eye damage/eye irritation

Shall not be classified as seriously damaging to the eye or eye irritant.

#### Respiratory or skin sensitisation

Shall not be classified as a respiratory or skin sensitiser.

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**Germ cell mutagenicity**

Shall not be classified as germ cell mutagenic.

**Carcinogenicity**

Shall not be classified as carcinogenic.

**Reproductive toxicity**

Shall not be classified as a reproductive toxicant.

**Specific target organ toxicity - single exposure**

Shall not be classified as a specific target organ toxicant (single exposure).

**Specific target organ toxicity - repeated exposure**

Shall not be classified as a specific target organ toxicant (repeated exposure).

**Aspiration hazard**

Shall not be classified as presenting an aspiration hazard.

**Symptoms related to the physical, chemical and toxicological characteristics**

• **If swallowed**

Data are not available.

• **If in eyes**

slightly irritant but not relevant for classification

• **If inhaled**

slightly irritant but not relevant for classification

• **If on skin**

slightly irritant but not relevant for classification

• **Other information**

none

**11.2 Endocrine disrupting properties**

Does not contain an endocrine disruptor (ED) at a concentration of  $\geq$  0,1%.

**11.3 Information on other hazards**

There is no additional information.

**SECTION 12: Ecological information**

**12.1 Toxicity**

Shall not be classified as hazardous to the aquatic environment.

Aquatic toxicity (acute)				
Endpoint	Value	Species	Source	Exposure time
LC50	6,7 mg/l	Pimephales promelas		96 h
EC50	27,1 mg/l	aquatic invertebrates	ECHA	48 h
ErC50	24,1 mg/l	algae	ECHA	72 h



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**12.2 Persistence and degradability**

Theoretical Oxygen Demand: 2,237 mg/mg

Theoretical Carbon Dioxide: 2,637 mg/mg

**Biodegradation**

The substance is readily biodegradable.

**Process of degradability**

Process	Degradation rate	Time
oxygen depletion	69 %	28 d

**12.3 Bioaccumulative potential**

Does not significantly accumulate in organisms.

n-octanol/water (log KOW)

2,59 (22,8 °C) (ECHA)

**12.4 Mobility in soil**

Data are not available.

**12.5 Results of PBT and vPvB assessment**

Data are not available.

**12.6 Endocrine disrupting properties**

Does not contain an endocrine disruptor (ED) at a concentration of  $\geq$  0,1%.

**12.7 Other adverse effects**

Data are not available.

**SECTION 13: Disposal considerations**

**13.1 Waste treatment methods**



Consult the appropriate local waste disposal expert about waste disposal.

**Sewage disposal-relevant information**

Do not empty into drains.

**Waste treatment of containers/packagings**

Handle contaminated packages in the same way as the substance itself. Completely emptied packages can be recycled.

**13.2 Relevant provisions relating to waste**

The allocation of waste identity numbers/waste descriptions must be carried out according to the EEC, specific to the industry and process.

**13.3 Remarks**

Waste shall be separated into the categories that can be handled separately by the local or national waste management facilities. Please consider the relevant national or regional provisions. Non-contaminated packages may be recycled.

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## SECTION 14: Transport information

- 14.1 UN number or ID number** not subject to transport regulations
- 14.2 UN proper shipping name** not assigned
- 14.3 Transport hazard class(es)** none
- 14.4 Packing group** not assigned
- 14.5 Environmental hazards** non-environmentally hazardous acc. to the dangerous goods regulations
- 14.6 Special precautions for user**  
There is no additional information.
- 14.7 Maritime transport in bulk according to IMO instruments**  
The cargo is not intended to be carried in bulk.
- 14.8 Information for each of the UN Model Regulations**
- International Maritime Dangerous Goods Code (IMDG) - Additional information**  
Not subject to IMDG.
- International Civil Aviation Organization (ICAO-IATA/DGR) - Additional information**  
Not subject to ICAO-IATA.

## SECTION 15: Regulatory information

- 15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture**
- Relevant provisions of the European Union (EU)**
- Restrictions according to REACH, Annex XVII**  
not listed
- List of substances subject to authorisation (REACH, Annex XIV)/SVHC - candidate list**  
Not listed.
- Seveso Directive**

2012/18/EU (Seveso III)			
No	Dangerous substance/hazard categories	Qualifying quantity (tonnes) for the application of lower and upper-tier requirements	Notes
	not assigned		

### Deco-Paint Directive

VOC content	100 %
VOC content	1.050 g/l

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## Industrial Emissions Directive (IED)

VOC content	100 %
VOC content	1.050 g/l

## Directive on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS)

not listed

## Regulation concerning the establishment of a European Pollutant Release and Transfer Register (PRTR)

not listed

## Water Framework Directive (WFD)

not listed

## Regulation on the marketing and use of explosives precursors

not listed

## Regulation on drug precursors

not listed

## Regulation on substances that deplete the ozone layer (ODS)

not listed

## Regulation concerning the export and import of hazardous chemicals (PIC)

not listed

## Regulation on persistent organic pollutants (POP)

not listed

## Other information

Directive 94/33/EC on the protection of young people at work. Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.

## National inventories

Country	Inventory	Status
AU	AIIC	substance is listed
CA	DSL	substance is listed
CN	IECSC	substance is listed
EU	ECSI	substance is listed
EU	REACH Reg.	substance is listed
JP	CSCL-ENCS	substance is listed
KR	KECI	substance is listed
MX	INSQ	substance is listed
NZ	NZIoC	substance is listed
PH	PICCS	substance is listed
TW	TCSI	substance is listed

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Country	Inventory	Status
US	TSCA	substance is listed (ACTIVE)
VN	NCI	substance is listed

### Legend

AIIC	Australian Inventory of Industrial Chemicals
CSCL-ENCS	List of Existing and New Chemical Substances (CSCL-ENCS)
DSL	Domestic Substances List (DSL)
EC SI	EC Substance Inventory (EINECS, ELINCS, NLP)
IECSC	Inventory of Existing Chemical Substances Produced or Imported in China
INSQ	National Inventory of Chemical Substances
KECI	Korea Existing Chemicals Inventory
NCI	National Chemical Inventory
NZIoC	New Zealand Inventory of Chemicals
PICCS	Philippine Inventory of Chemicals and Chemical Substances (PICCS)
REACH Reg.	REACH registered substances
TCSI	Taiwan Chemical Substance Inventory
TSCA	Toxic Substance Control Act

## 15.2 Chemical safety assessment

No Chemical Safety Assessment has been carried out for this substance.

## SECTION 16: Other information

### Indication of changes (revised safety data sheet)

Section	Former entry (text/value)	Actual entry (text/value)	Safety-relevant
2.3		Endocrine disrupting properties: Does not contain an endocrine disruptor (ED) at a concentration of $\geq$ 0,1%.	yes
14.8	Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN) - Additional information: Not subject to ADR, RID and ADN.		yes
15.1	VOC content: 100 % 1.050 g/l	VOC content: 100 %	yes
15.1		VOC content: 1.050 g/l	yes
15.1		National inventories: change in the listing (table)	yes

### Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
ADR	Accord relatif au transport international des marchandises dangereuses par route (Agreement concerning the International Carriage of Dangerous Goods by Road)
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
CLP	Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures
DGR	Dangerous Goods Regulations (see IATA/DGR)
DNEL	Derived No-Effect Level
EC50	Effective Concentration 50 %. The EC50 corresponds to the concentration of a tested substance causing 50 % changes in response (e.g. on growth) during a specified time interval

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Abbr.	Descriptions of used abbreviations
EC No	The EC Inventory (EINECS, ELINCS and the NLP-list) is the source for the seven-digit EC number, an identifier of substances commercially available within the EU (European Union)
ED	Endocrine disruptor
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
ErC50	$\equiv$ EC50: in this method, that concentration of test substance which results in a 50 % reduction in either growth (EbC50) or growth rate (ErC50) relative to the control
GHS	"Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Nations
IATA	International Air Transport Association
IATA/DGR	Dangerous Goods Regulations (DGR) for the air transport (IATA)
ICAO	International Civil Aviation Organization
IMDG	International Maritime Dangerous Goods Code
LC50	Lethal Concentration 50%: the LC50 corresponds to the concentration of a tested substance causing 50 % lethality during a specified time interval
LD50	Lethal Dose 50 %: the LD50 corresponds to the dose of a tested substance causing 50 % lethality during a specified time interval
LEL	Lower explosion limit (LEL)
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No-Effect Concentration
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SVHC	Substance of Very High Concern
VOC	Volatile Organic Compounds
vPvB	Very Persistent and very Bioaccumulative

### Key literature references and sources for data

Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures.  
Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU.

Agreement concerning the International Carriage of Dangerous Goods by Road (ADR). International Maritime Dangerous Goods Code (IMDG). Dangerous Goods Regulations (DGR) for the air transport (IATA).

### Disclaimer

This information is based upon the present state of our knowledge. This SDS has been compiled and is solely intended for this product.