

4-Hydroxybenzoic acid propyl ester ≥98 %, Ph.Eur., USP

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Replaces version of: 10.08.2021

Version: (1)

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

1.1 **Product identifier**

Identification of the substance **4-Hydroxybenzoic acid propyl ester** ≥98 %,

Ph.Ěur., UŠP

Article number 6882

Registration number (REACH) 01-2119969462-29-XXXX

EC number 202-307-7 CAS number 94-13-3

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 **Telefax:** +49 (0) 721 - 56 06 149 e-mail: sicherheit@carlroth.de Website: www.carlroth.de

sheet:

sicherheit@carlroth.de e-mail (competent person):

1.4 **Emergency telephone number**

SECTION 2: Hazards identification

Classification of the substance or mixture 2.1

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

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2.3 Other hazards

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

The substance has an endocrine disrupting potential.

SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance 4-Hydroxybenzoic acid propyl ester

Molecular formula $C_{10}H_{12}O_3$ Molar mass $180,2\,^g/_{mol}$

REACH Reg. No 01-2119969462-29-XXXX

CAS No 94-13-3 EC No 202-307-7

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

Symptoms and effects are not known to date.

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, foam, dry extinguishing powder, ABC-powder

Unsuitable extinguishing media

water jet

5.2 Special hazards arising from the substance or mixture

Combustible.

Hazardous combustion products

In case of fire may be liberated: Carbon monoxide (CO), Carbon dioxide (CO₂)

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

Control of dust.

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. Take up mechanically.

Advice on how to clean up a spill

Take up mechanically.

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.

Advice on general occupational hygiene

Keep away from food, drink and animal feedingstuffs.

7.2 Conditions for safe storage, including any incompatibilities

Store in a dry place.

Incompatible substances or mixtures

Observe hints for combined storage.

Consideration of other advice:

Ventilation requirements

Use local and general ventilation.

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 DNE	Relevant DNELs and other threshold levels					
Endpoint	Threshold level	Protection goal, route of exposure	Used in	Exposure time		
DNEL	88,2 mg/m³	human, inhalatory	worker (industry)	chronic - systemic effects		
DNEL	675,6 mg/kg bw/day	human, dermal	worker (industry)	chronic - systemic effects		

Environmental values

Relevant	Relevant PNECs and other threshold levels						
End- point	Threshold Organism level		Environmental com- partment	Exposure time			
PNEC	0,0206 ^{mg} / _{cm³}	unknown	marine sediment	intermittent release			
PNEC	0,00064 ^{mg} / _{cm³}	unknown	marine water	intermittent release			
PNEC	0,064 ^{mg} / _{cm³}	unknown	air	intermittent release			
PNEC	0,2065 ^{mg} / _{cm³}	unknown	freshwater sediment	intermittent release			

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Relevant PNECs and other threshold levels							
End- Threshold point level		Organism	Environmental com- partment	Exposure time			
PNEC	0,0064 ^{mg} / _{cm³}	unknown	freshwater	intermittent release			
PNEC	0,0375 ^{mg} / _{cm³}	unknown	soil	intermittent release			
PNEC	0,017 ^{mg} / _l	aquatic organisms	freshwater	short-term (single instance)			
PNEC	0,002 ^{mg} / _l	aquatic organisms	marine water	short-term (single instance)			
PNEC	2 ^{mg} / _l	aquatic organisms	sewage treatment plant (STP)	short-term (single instance)			
PNEC	0,115 ^{mg} / _{kg}	aquatic organisms	freshwater sediment	short-term (single instance)			
PNEC	0,011 ^{mg} / _{kg}	aquatic organisms	marine sediment	short-term (single instance)			
PNFC	0.052 ^{mg} / _{lea}	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

NBR (Nitrile rubber)

material thickness

>0,11 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





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Respiratory protection necessary at: Dust formation. Particulate filter device (EN 143). P1 (filters at least 80 % of airborne particles, colour code: White).

Environmental exposure controls

Keep away from drains, surface and ground water.

SECTION 9: Physical and chemical properties

Information on basic physical and chemical properties 9.1

Physical state solid

Form powder, crystalline

Colour white

Odour characteristic 96 - 98 °C Melting point/freezing point 301 °C (ECHA)

Boiling point or initial boiling point and boiling

range

this material is combustible, but will not ignite **Flammability**

readily

Lower and upper explosion limit not determined

Flash point 180°C

Auto-ignition temperature not determined Decomposition temperature not relevant

pH (value) 7 (in aqueous solution: 0,4 ^g/_I, 20 °C)

Kinematic viscosity not relevant

Solubility(ies)

Water solubility $0.5 \,^{\mathrm{g}}$ /_I at 25 °C (TOXNET)

Partition coefficient

Partition coefficient n-octanol/water (log value): 3,04 (exp. (TOXNET))

Soil organic carbon/water (log KOC) 2,457 (ECHA)

0 Pa at 20 °C Vapour pressure

Density and/or relative density

 $1,287 \, {}^{9}/_{cm^{3}}$ at 20 °C (ECHA) Density

Relative vapour density Information on this property is not available.

 $\sim 350 \, \text{kg/m}^3$ **Bulk density**

No data available. Particle characteristics

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Other safety parameters

Oxidising properties none

9.2 Other information

Information with regard to physical hazard

classes:

hazard classes acc. to GHS (physical hazards): not relevant

Other safety characteristics:

Temperature class (EU, acc. to ATEX)

Maximum permissible surface temperature on

the equipment: 450°C

SECTION 10: Stability and reactivity

10.1 Reactivity

The product in the delivered form is not dust explosion capable; the enrichment of fine dust however leads to the danger of dust explosion.

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

10.4 Conditions to avoid

There are no specific conditions known which have to be avoided.

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

Exp	osure route	Endpoint	Value	Species	Method	Source
	oral	LD50	>5.000 ^{mg} / _{kg}	rat		ECHA

Skin corrosion/irritation

Shall not be classified as corrosive/irritant to skin.

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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.

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

Data are not available.

If inhaled

Data are not available.

• If on skin

Data are not available.

Other information

Health effects are not known.

11.2 Endocrine disrupting properties

This substance is known as an "endocrine disruptor".

Endocrine disrupting chemicals (EDC)

Name of substance	CAS No	Combined cat- egory	Human health category	Wildlife cat- egory
4-Hydroxybenzoic acid propyl ester	94-13-3	CAT1	CAT1	CAT1

Legend

CAT1 Category 1 - evidence of endocrine disruption in at least one species using intact animals

11.3 Information on other hazards

There is no additional information.

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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	6,4 ^{mg} / _l	fish	ECHA	96 h
EC50	15,4 ^{mg} / _l	aquatic invertebrates	ECHA	48 h
ErC50	16 ^{mg} / _l	algae	ECHA	72 h

12.2 Persistence and degradability

Theoretical Oxygen Demand: $2,042 \frac{mg}{mg}$ /_{mg} Theoretical Carbon Dioxide: $2,442 \frac{mg}{mg}$ /_{mg}

Biodegradation

The substance is readily biodegradable.

Process of degradability

Process	Degradation rate	Time
biotic/abiotic	>90 %	d
oxygen depletion	91,5 %	28 d

12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW)	3,04 (Exp. (TOXNET))
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12.4 Mobility in soil

The Organic Carbon normalised adsorption coefficient	2,457 (ECHA)
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12.5 Results of PBT and vPvB assessment

Data are not available.

12.6 Endocrine disrupting properties

This substance is known as an "endocrine disruptor".

Endocrine disrupting chemicals (EDC)

Name of substance	CAS No	Combined cat- egory	Human health category	Wildlife cat- egory
4-Hydroxybenzoic acid propyl ester	94-13-3	CAT1	CAT1	CAT1

Legend

CAT1 Category 1 - evidence of endocrine disruption in at least one species using intact animals

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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.

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 dan-

gerous 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.

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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	0 %
VOC content	0 ^g / _l

Industrial Emissions Directive (IED)

VOC content	0 %
VOC content	0 ^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)

List of pollutants (WFD) Name of substance **CAS No** Listed in **Remarks** Name acc. to inventory 4-Hydroxybenzoic acid propyl es-Substances and preparations, or a) the breakdown products of such, which have been proved to possess carcinogenic or mutagenic properties or properties which may affect steroidogenic, thyroid, reproduction or other endocrinerelated functions in or via the aquatic environment

Legend

a) Indicative list of the main pollutants

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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
JP	ISHA-ENCS	substance is listed
KR	KECI	substance is listed
MX	INSQ	substance is listed
NZ	NZIoC	substance is listed
PH	PICCS	substance is listed
TR	CICR	substance is listed
TW	TCSI	substance is listed
US	TSCA	substance is listed (ACTIVE)
VN	NCI	substance is listed

Legend

AIIC CICR Australian Inventory of Industrial Chemicals

Chemical Inventory and Control Regulation List of Existing and New Chemical Substances (CSCL-ENCS)

CSCL-ENCS DSL ECSI IECSC

Domestic Substances List (DSL)
EC Substance Inventory (EINECS, ELINCS, NLP)
Inventory of Existing Chemical Substances Produced or Imported in China National Inventory of Chemical Substances

Inventory of Existing and New Chemical Substances (ISHA-ENCS) 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

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Legend

TSCA Toxic Substance Control Act

15.2 Chemical safety assessment

According to REACH, Article 14 (1) a chemical safety assessment has been carried out for this substance or components of this mixture when the substance has been registered in quantities of 10 tonnes or more per year per registrant.

SECTION 16: Other information

Indication of changes (revised safety data sheet)

Section	Former entry (text/value)	Actual entry (text/value)	Safety- relev- ant
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: 0 % 0 ^g / ₁	VOC content: 0 %	yes
15.1		VOC content: 0 ^g / _l	yes
15.1		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.	yes
15.1		National inventories: change in the listing (table)	yes
15.2	Chemical Safety Assessment: No Chemical Safety Assessment has been car- ried out for this substance.	Chemical safety assessment: According to REACH, Article 14 (1) a chemical safety assessment has been carried out for this substance or components of this mixture when the substance has been registered in quantities of 10 tonnes or more per year per registrant.	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
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)
EINECS	European Inventory of Existing Commercial Chemical Substances

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Abbr.	Descriptions of used abbreviations
ELINCS	European List of Notified Chemical Substances
ErC50	≡ 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
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.

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