



Safety data sheet according to 1907/2006/EC, Article 31

Printing date 25.03.2011

Version number 3

Revision: 25.03.2011

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

- Product identifier

- **Trade name:** para-Hydroxybenzoic acid (pHBA)

- **CAS number:**

99-96-7

- **EINECS number:**

202-804-9

- **Registration number** 01-2119487280-38-0000

- **Relevant identified uses of the substance or mixture and uses advised against**

PROC 4: Use in batch and other process (synthesis) where opportunity for exposure arises.

Market sector by type of chemical product:

PC 19: Intermediate

- **Application of the substance / the preparation -**

- Details of the supplier of the safety data sheet

- **Manufacturer/Supplier:**

LCP Leuna Carboxylation Plant GmbH

Am Haupttor

06237 Leuna

Tel. : +49 (3461) 43 43 50

Fax : + 49 (3461) 43 43 52

- **Further information obtainable from:** info@lcp-carboxy.com

- **Emergency telephone number:** + 49 (3461) 43 43 33 (Plant fire Dept. at chemical site Leuna)

2 Hazards identification

- Classification of the substance or mixture

- **Classification according to Regulation (EC) No 1272/2008**



GHS05 corrosion

Eye Dam. 1 H318 Causes serious eye damage.



GHS07

STOT SE 3 H335 May cause respiratory irritation.

- **Classification according to Directive 67/548/EEC or Directive 1999/45/EC**



Xi; Irritant

R37-41: Irritating to respiratory system. Risk of serious damage to eyes.

- Label elements

- **Labelling according to Regulation (EC) No 1272/2008**

The substance is classified and labelled according to the CLP regulation.

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- Hazard pictograms

GHS05 GHS07

- Signal word Danger**- Hazard statements**

H318 Causes serious eye damage.

H335 May cause respiratory irritation.

- Precautionary statements

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P310 Immediately call a POISON CENTER or doctor/physician.

P405 Store locked up.

P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

- Other hazards**- Results of PBT and vPvB assessment**- **PBT:** Not applicable.- **vPvB:** Not applicable.

3 Composition/information on ingredients

- Chemical characterization: Substances**- CAS No. Description**

99-96-7 4-Hydroxybenzoic acid

- Identification number(s)

- EINECS Number: 202-804-9

4 First aid measures

- Description of first aid measures- **General information:** Immediately remove any clothing soiled by the product.- **After inhalation:** In case of unconsciousness place patient stably in side position for transportation.- **After skin contact:** Immediately wash with water and soap and rinse thoroughly.**- After eye contact:**

Rinse opened eye for several minutes under running water. If symptoms persist, consult a doctor.

- **After swallowing:** Do not induce vomiting; call for medical help immediately.- **Information for doctor:** symptomatic treatment and if possible contact poison specialist.

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5 Firefighting measures

- **Extinguishing media**
 - **Suitable extinguishing agents:**
CO₂, powder or water spray. Fight larger fires with water spray or alcohol resistant foam.
- **Special hazards arising from the substance or mixture**
Carbon monoxide (CO)
Formation of toxic gases is possible during heating or in case of fire.
- **Advice for firefighters**
 - **Protective equipment:** Wear self-contained respiratory protective device.
- **Additional information** Cool endangered receptacles with water spray.

6 Accidental release measures

- **Personal precautions, protective equipment and emergency procedures**
Ensure adequate ventilation.
Wear protective equipment. Keep unprotected persons away.
- **Environmental precautions:** Do not allow to enter sewers/ surface or ground water.
- **Methods and material for containment and cleaning up:**
Pick up mechanically.
Send for recovery or disposal in suitable receptacles.
- **Reference to other sections**
See Section 7 for information on safe handling.
See Section 13 for disposal information.

7 Handling and storage

- **Handling:**
 - **Precautions for safe handling**
Ensure good ventilation/exhaustion at the workplace.
Store in cool, dry place in tightly closed receptacles.
 - **Information about fire - and explosion protection:** The product is not flammable.
- **Conditions for safe storage, including any incompatibilities**
 - **Storage:**
 - **Requirements to be met by storerooms and receptacles:**
Avoid dust clouds to come into contact with ignition sources e.g. sparks.
Use only big bags equipped with conductivity for electrostatic discharge.
Earthing of big bags required for filling and emptying. Store in a dry place.
Keep away from sources of ignition and strong oxidizing agents.
DO NOT USE FOOD CONTAINERS. RISK OF CONFUSION!
Containers are clearly and permanently labelled.
Store in the original container if possible. Keep container tightly closed.
Keep container well below 150°C.
Storage temperature: well below 150°C
 - **Information about storage in one common storage facility:**
CAUTION
Store away from oxidizing agents.

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- **Further information about storage conditions:** -
- **Storage class:** VCI Storage category: 10-13

8 Exposure controls/personal protection

- **Additional information about design of technical facilities:** No further data; see item 7.
- **Control parameters**
 - **Ingredients with limit values that require monitoring at the workplace:** Not required.
 - **DNELs**
Inhalation: 2.4 mg/m³
Dermal: 8.6 mg/cm²
No other DNELs relevant because of substance properties Uses and exposures.
 - **PNECs**
PNEC aqua (freshwater)
2 mg/L
PNEC STP
1.1 mg/L
No other PNECs relevant because of substance properties Uses and exposures.
 - **Additional information:** The lists valid during the making were used as basis.
- **Exposure controls**
 - **Personal protective equipment:**
 - **General protective and hygienic measures:**
Keep away from foodstuffs, beverages and feed.
Immediately remove all soiled and contaminated clothing
Wash hands before breaks and at the end of work.
Avoid contact with the eyes and skin.
 - **Respiratory protection:**
In case of brief exposure or low pollution use respiratory filter device. In case of intensive or longer exposure use self-contained respiratory protective device.
 - **Protection of hands:**



Protective gloves

The glove material has to be impermeable and resistant to the substance.
Selection of the glove material on consideration of the penetration times, rates of diffusion and the degradation

- **Material of gloves**
The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer.
- **Penetration time of glove material**
The exact break through time has to be found out by the manufacturer of the protective gloves and has to be observed.

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- Eye protection:

Tightly sealed goggles

- Body protection: Protective work clothing

9 Physical and chemical properties

- Information on basic physical and chemical properties

- General Information

- Appearance:**- Form:** Powder**- Colour:** White**- Odour:** Odourless**- pH-value (1 g/l) at 20°C:** 3.3 (Company data)

- Change in condition

- Melting point/Melting range: 215-216°C (OECD 102 resp. EU A1)**- Boiling point/Boiling range:** The study is not necessary and scientifically unjustified because p-hydroxybenzoic acid (the substance) decomposes before boiling.

- Flash point:

pHBA is solid at room temperature. The flash point is only a relevant property for liquids, thus it does not need to be done for substances that are solids (as described in the endpoint specific guidance CHAPTER R.7A of ECHAs Guidance on information requirements and chemical safety assessment).

- Flammability (solid, gaseous): Product is considered not flammable.**- Danger of explosion:** Product does not present an explosion hazard.

- Explosion limits:

- Oxidizing properties

The substance is incapable of reacting exothermically with combustible materials on the basis of the chemical structure.

None of the common chemical groups associated with oxidising properties is present in p-hydroxybenzoic acid

- Vapour pressure:

at 20 °C $1.05 \cdot 10^{-7}$ hPaat 25 °C $2.11 \cdot 10^{-7}$ hPa

(OECD 104, resp. EU A.4)

- Density:

- Relative density 1,404 (OECD 109/EU A.3)

- Solubility in / Miscibility with

- water: at 20 °C 4,87g/l (OECD 105)

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- **Viscosity:**
 - **Dynamic:** This study is technically not feasible and scientifically unjustified, because para-hydroxybenzoic acid is a solid up to 215 °C.
- **Other information** Para-hydroxybenzoic acid is stable in dimethyl sulfoxide (DMSO) according to a study at 20 °C for a 14 days period.
Para-hydroxybenzoic acid is stable in diisopropylether (DIPE)

10 Stability and reactivity

- **Reactivity**
 - **Chemical stability**
 - **Thermal decomposition / conditions to be avoided:**
Thermal decomposition starting slowly at 200 °C. Keep temperature at least at safety margin according to TRAS 410 (Technische Regel Anlagesicherheit) (e.g. 50 K below 200°C)
 - **Possibility of hazardous reactions** See above
 - **Incompatible materials:** Keep away from oxidising agents and acidic substances.
 - **Hazardous decomposition products:**
Phenol
Carbon monoxide and carbon dioxide

11 Toxicological information

- Information on toxicological effects**- Acute toxicity:****- LD/LC50 values relevant for classification:**

Oral	LD ₅₀	> 2000 mg/kg bw. (rat) (S. Colas 2009; OECD 423)
Dermal	LD ₅₀	> 2000 mg/kg bw. (rabbit) (Carol S. Auletta; 1981)
Inhalative	LD ₅₀ /4h(dust)	0.47 mg/L (analytical). (rat) (Davis (1980)) 7.91 mg/L (nominal) (rat) (Davis (1980))

- Primary irritant effect:**- on the skin:**

No irritant effect.

irritating effect on mucous membranes (NOEC (respiratory irritation) = 60 mg/m³, 11 d inhalation study with repeated doses, rat) , Roger Ben Dyke (1981)**- on the eye:**

corrosivity:

corrosive to eyes (rabbit) (OECD Guideline 405) , F. Richeux (2010)

- Sensitization:

not sensitising (guinea pig (Buehler test) Auletta (1981), mouse (Local lymph node assay, OECD Guideline 429 Honorvar N (2009)

- Additional toxicological information:

not regarded as genotoxic.

bacterial reverse mutation assay (Ames test, OECD 471): negative
(Paulus, 2009)

in vitro mammalian chromosome aberration test (Chromosome aberration):

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negative (Nohiro Tanaka et al., 1997)

- Toxicokinetics, metabolism and distribution**-after oral administration:**

4-HBA is resorbed relatively fast and it is relatively fast excreted with the urine. No accumulation was observed. Relevant parts of the resorbed substance are excreted unchanged. Main metabolite: glucuronic acid conjugate (human, dog).

-Dermal:

Dermal absorption study (female rat, occlusive coverage, 120 h):

Result: 4 % absorption. Obviously 4-HBA is not resorbed through the intact skin in relevant amounts.

- Repeated dose toxicity

Repeated dose inhalation:

NOEC (local effects): 60 mg/m³ (6 h, rat).

combined repeated dose and reproduction / developmental screening (oral: gavage, OECD Guideline 422): NOEL (developmental/ teratogenic and fertility parameters): 1000 mg/kg bw/day (Tetsuji Nagao et al. (1997))

No teratogenicity was observed in studies with methyl parabene (rat, mouse, hamster (FDRL (Food and Drug Research Labs) (1972)), rabbit (FDRL) (Food and Drug Research Labs) (1973)). Pharmacokinetic investigations showed that methyl parabene is transformed to 4-HBA in the body. Therefore, these studies can be used to assess teratogenicity of 4-HBA.

Repeated dose toxicity (other routes):

mouse (subacute (subcutaneous)) NOEL: \geq 100 mg/kg bw/day (no effects on body weight, no clinical signs (Twomey, K (2000a))**- CMR effects (carcinogenicity, mutagenicity and toxicity for reproduction)**

Carcinogenic potential:

Two longterm studies one with rats another one with dogs with Methyl-4-hydroxy benzoate revealed no hints for a carcinogenic potential of 4-HBA (Matthews et al. 1956). Pharmacokinetic investigations showed that Methyl-4-hydroxy benzoate is transformed to 4-HBA in the body. Therefore, these studies can be used to assess carcinogenic effects of 4-HBA.

12 Ecological information

- Toxicity**- Aquatic toxicity:**

EC ₅₀ /48h	67 mg/L without pH adjustment (D. subspicatus) (OECD 202, Biermann, (2009a)) > 1000mg/L neutral pH, (Daphnia magna) (OECD 202, Biermann, (2009a))
ErC ₅₀ /72h	92 mg/L without pH adjustment (D. subspicatus) (OECD 201, Biermann, (2009b)) > 1000 mg/L pH adjustment to 7.5 (D. subspicatus) (OECD 201, Biermann, (2009b))
LC ₅₀ /14d	66.5 mg /L without pH adjustment (Oryzias latipes) (OECD 204) > 100 mg/L (Oryzias latipes) (OECD 204, neutral pH, T. Research center (1997))
LC ₅₀ /96h	92.8 mg/L without pH adjustment (Oryzias latipes) (OECD 203) > 100 mg/L pH =6.7 (Oryzias latipes) (OECD 203; T. Research center Inc. (1997a))
NOEC/21d	100 mg/L non-neutralized pH (Daphnia magna) (OECD 202, Toray Research Center Tokyo (1997b))

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- Behaviour in environmental systems:**- Bioaccumulative potential**

log K (o/w)= 0,88 (22 °C, pH 3,5, non-ionised for m)

Due to the distribution coefficient n-octanol/water an accumulation in organisms is not expected.

- Additional ecological information:**- General notes:**

Water hazard class 1 (German Regulation) (Assessment by list): slightly hazardous for water

Do not allow undiluted product or large quantities of it to reach ground water, water course or sewage system.

- Results of PBT and vPvB assessment**- PBT:** Not applicable.**- vPvB:** Not applicable.

13 Disposal considerations

- Waste treatment methods**- Recommendation**

Must not be disposed together with household garbage. Do not allow product to reach sewage system.

- Uncleaned packaging:**- Recommendation:** Disposal must be made according to official regulations.

14 Transport information

- Land transport ADR/RID (cross-border)**- ADR/RID class:** -**- Danger code (Kemler):** -**- UN-Number:****- Packaging group:** -**- Hazard label:** -**- UN proper shipping name:****- Limited quantities (LQ)** -**- Remarks:** Not regulated as a dangerous good**- Maritime transport IMDG:****- IMDG Class:** -**- UN Number:** -

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- **Label** -
- **EMS Number:** -
- **Marine pollutant:** No
- **Remarks:** Not regulated as a dangerous good

- Air transport ICAO-TI and IATA-DGR:

- **ICAO/IATA Class:** -
- **UN/ID Number:** -
- **Label** -
- **Packaging group:** -

- **UN "Model Regulation":** -
- **Special precautions for user** Not applicable.
- **Transport/Additional information:** Not dangerous according to the above specifications.

15 Regulatory information

- **Chemical safety assessment:** A Chemical Safety Assessment has been carried out.

16 Other information

This information is based on our present knowledge. However, this shall not constitute a guarantee for any specific product features and shall not establish a legally valid contractual relationship.

- **Department issuing MSDS:** Product Safety Departement

- Contact:

+ 49 (3461) 43 43 33

only available during office hours.

- Abbreviations and acronyms:

EC50: effective concentration, 50 percent

ADR: Accord européen sur le transport des marchandises dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by Road)

RID: Règlement international concernant le transport des marchandises dangereuses par chemin de fer (Regulations Concerning the International Transport of Dangerous Goods by Rail)

IMDG: International Maritime Code for Dangerous Goods

IATA: International Air Transport Association

IATA-DGR: Dangerous Goods Regulations by the "International Air Transport Association" (IATA)

ICAO: International Civil Aviation Organization

ICAO-TI: Technical Instructions by the "International Civil Aviation Organization" (ICAO)

GHS: Globally Harmonized System of Classification and Labelling of Chemicals

EINECS: European Inventory of Existing Commercial Chemical Substances

CAS: Chemical Abstracts Service (division of the American Chemical Society)

DNEL: Derived No-Effect Level (REACH)

PNEC: Predicted No-Effect Concentration (REACH)

LC50: Lethal concentration, 50 percent

LD50: Lethal dose, 50 percent

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