

Chemical Safety Data Sheet MSDS / SDS

4-hydroxybenzoic acid SDS

Revision Date:2024-04-25 Revision Number:1

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

Product name: 4-hydroxybenzoic acid

CAS: 99-96-7

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

Relevant identified uses: For R&D use only. Not for medicinal, household or other use.

Uses advised against: none

Company Identification

Company: Chemicalbook.in

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SECTION 2: Hazards identification**Classification of the substance or mixture**

Serious eye damage, Category 1

Specific target organ toxicity - single exposure, Category 3

Specific target organ toxicity - single exposure, Category 3

GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Danger

Hazard statement(s)

H318 Causes serious eye damage

H335 May cause respiratory irritation

Precautionary statement(s)

Prevention

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

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

P271 Use only outdoors or in a well-ventilated area.

Response

P305+P354+P338 IF IN EYES: Immediately rinse with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P317 Get medical help.

P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.

P319 Get medical help if you feel unwell.

Storage

P403+P233 Store in a well-ventilated place. Keep container tightly closed.

P405 Store locked up.

Disposal

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

Other hazards which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

Substance

Chemical name:	4-hydroxybenzoic acid
Common names and synonyms:	4-hydroxybenzoic acid
CAS number:	99-96-7
EC number:	202-804-9
Concentration:	100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately. Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

Following skin contact

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

Following eye contact

Rinse with pure water for at least 15 minutes. Consult a doctor.

Following ingestion

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

Most important symptoms/effects, acute and delayed

no data available

Indication of immediate medical attention and special treatment needed, if necessary

Absorption, Distribution and Excretion

Groups of 4-8 rabbits were given 4-hydroxybenzoic acid at a dose of 100, 250, 500, 1000, or 1500 mg/kg bw by gavage every 3-7 days. Urine was collected continuously and analysed for metabolites. The total urinary recovery of the test material ranged from 84% to 104%. Glucuronic acid and sulfate conjugates were also detected in the urine, at 10-35% and 4-7%, respectively. The concentrations of all the metabolites returned to background values within 24 hr after dosing.

SECTION 5: Firefighting measures

Suitable extinguishing media

Use dry chemical, carbon dioxide or alcohol-resistant foam.

Specific hazards arising from the chemical

no data available

Special protective actions for fire-fighters

Wear self-contained breathing apparatus for firefighting if necessary.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

Environmental precautions

Prevent further spillage or leakage if it is safe to do so. Do not let the chemical enter drains. Discharge into the environment must be avoided.

Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

SECTION 7: Handling and storage

Precautions for safe handling

Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

Conditions for safe storage, including any incompatibilities

Store the container tightly closed in a dry, cool and well-ventilated place. Store apart from foodstuff containers or incompatible materials.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

no data available

Biological limit values

no data available

Appropriate engineering controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

Individual protection measures, such as personal protective equipment (PPE)

Eye/face protection

Wear tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

Skin protection

Wear fire/flame resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state:	Solid. Powder.
Colour:	White.
Odour:	no data available
Melting point/freezing point:	≥ 215.5 - ≤ 216.6 °C. Atm. press.:Ca. 1 atm.
Boiling point or initial boiling point and boiling range:	214°C(lit.)
Flammability:	no data available
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	88°C(lit.)
Auto-ignition temperature:	no data available
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	no data available
Solubility:	Solubility (in 100 g of solution): 99% ethanol 38.75 g (67 deg C); n-butanol 19.5 g (32.5 deg C)

Partition coefficient n-octanol/water:	$\log P_{ow} = 0.878$. Temperature: 22 °C.
Vapour pressure:	0 Pa. Temperature: 25 °C. Remarks: At 20 °C the vapour pressure is: 0.0000105 Pa; Based on measurements from 320 to 119.85 °C the following equation can be applied: $\log(p) = -5281.1 \times (1/T) + 13.038$ (p= vapour pressure in Pa); T = temperature in K.
Density and/or relative density:	> 1.34 - < 1.46. Temperature: 20 °C.
Relative vapour density:	no data available
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

no data available

Chemical stability

no data available

Possibility of hazardous reactions

no data available

Conditions to avoid

no data available

Incompatible materials

no data available

Hazardous decomposition products

When heated to decomposition it emits acrid smoke and irritating fumes.

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 Mouse oral 2200 mg/kg

Inhalation: discriminating conc. - rat (male/female) - ≥ 0.47 mg/L air (analytical).

Dermal: no data available

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

no data available

Reproductive toxicity

no data available

STOT-single exposure

no data available

STOT-repeated exposure

no data available

Aspiration hazard

no data available

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LC50 - *Oryzias latipes* - 92.8 mg/L - 96 h. Remarks: / without pH adjustment, pH = 4.0 to 4.5.

Toxicity to daphnia and other aquatic invertebrates: EC50 - *Daphnia magna* - 67 mg/L - 48 h. Remarks: / test without pH adjustment.

Toxicity to algae: EC50 - *Desmodesmus subspicatus* (previous name: *Scenedesmus subspicatus*) - 92 mg/L - 72 h.

Toxicity to microorganisms: MIC = Minimal Inhibitory Concentration - *Escherichia coli* - 8.2 mmol/L - 24 h.

Persistence and degradability

AEROBIC: In a 1% soil suspension screening test, 4-hydroxybenzoic acid at 25 ppm was completely degraded within 1 day, as measured by loss of UV absorbancy(1). 4-Hydroxybenzoic acid was readily biodegraded in several aerobic activated sludge screening tests including the Zahn-Wellens test (100% removal in 1 day), Japanese MITI test (98% theoretical BOD reached in 14 days), Sturm CO₂ evolution test (61% theoretical CO₂ produced in 28 days), OECD Screening test (95% DOC removal in 19 days), and the Closed bottle test (93% theoretical BOD reached in 30 days)(2). In an OECD coupled units biological treatment simulation test, 99% DOC removal of 4-hydroxybenzoic acid, initially present at 12 ppm C, was reported after an acclimation period of 7 days(2). 4-Hydroxybenzoic acid was mineralized 44 to 54% in 14 days in an assay where aquifer sediments from outside the coal-tar contaminated plume were added to the compound in distilled water at 20 deg C(3). When aquifer sediment collected from within the plume were used, from 50 to over 80% of the added 4-hydroxybenzoic acid was generally mineralized within 14 days(3). Under microaerophilic conditions, mineralization of 4-hydroxybenzoic acid ranged from 13 to 54% in 6 days; sediment collected from within the plume was used as an inoculum(3). Under aerobic conditions, using the same sediment, from 34 to 70% mineralization was reported over the same time(3). The percent 4-hydroxybenzoic acid mineralization in 20 days ranged from 35 to 55, 35 to 55, and 0 to 35 in microcosms using sediment upgradient of a coal-tar contaminated plume, downgradient of the plume, and in pristine sediment, respectively(4). Mineralization of 4-hydroxybenzoic acid in aquifer sediment microcosms from uncontaminated and contaminated boreholes in an urban coal-tar waste site was reported as 43 to 51% and 46 to 52%, respectively, in 14 days(5).

Bioaccumulative potential

An estimated BCF of 9 was calculated for 4-hydroxybenzoic acid(SRC), using a log Kow of 1.58(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is

low(SRC), provided the compound is not altered physically or chemically once released into the environment.

Mobility in soil

Koc values of 142, 20, and 14 were measured according to a modified version of OECD guideline 106 for 4-hydroxybenzoic acid in a podzol (pH=2.8, C organic=4.85%, sand:silt:clay=89.2:8.2:2.6%), alfisol (pH=6.7, C organic=1.25%, sand:silt:clay=69.7:14.4:15.9%), and a sediment (pH=7.1, C organic=1.58%, sand:silt:clay=5.5:58.8:35.7%), respectively(1). According to a classification scheme(2), these Koc values suggest that 4-hydroxybenzoic acid is expected to have high to very high mobility in soil. The pKa of 4-hydroxybenzoic acid is 4.54(3), indicating that this compound will primarily exist in anion form in the environment and anions generally do not adsorb more strongly to organic carbon and clay than their neutral counterparts(4).

Other adverse effects

no data available

SECTION 13: Disposal considerations

Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

UN Number

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: Not dangerous goods. (For reference only, please check.)
IMDG: Not dangerous goods. (For reference only, please check.)
IATA: Not dangerous goods. (For reference only, please check.)

Transport hazard class(es)

ADR/RID: Not dangerous goods. (For reference only, please check.)
IMDG: Not dangerous goods. (For reference only, please check.)
IATA: Not dangerous goods. (For reference only, please check.)

Packing group, if applicable

ADR/RID: Not dangerous goods. (For reference only, please check.)
IMDG: Not dangerous goods. (For reference only, please check.)
IATA: Not dangerous goods. (For reference only, please check.)

Environmental hazards

ADR/RID: No
IMDG: No
IATA: No

Special precautions for user

no data available

Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

Safety, health and environmental regulations specific for the product in question

European Inventory of Existing Commercial Chemical Substances (EINECS)

Listed.

EC Inventory

Listed.

United States Toxic Substances Control Act (TSCA) Inventory

Listed.

China Catalog of Hazardous chemicals 2015

Not Listed.

New Zealand Inventory of Chemicals (NZIoC)

Listed.

(PICCS)

Listed.

Vietnam National Chemical Inventory

Listed.

IECSC)

Listed.

Korea Existing Chemicals List (KECL)

Listed.

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

References

IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:
http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

ERG - Emergency Response Guidebook by U.S. Department of Transportation, website:
<http://www.phmsa.dot.gov/hazmat/library/erg>

Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

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