

Safety Data Sheet

according to Regulation (EC) No 1907/2006

4-Nitrobenzoic Acid

Revision: 29.01.2025

Product code: AC15.03758

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

1.1. Product identifier

4-Nitrobenzoic Acid

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

Use of the substance/mixture

Reagents and laboratory chemicals
Only for laboratory and analysis purposes.

Uses advised against

Do not use for private purposes (household).

1.3. Details of the supplier of the safety data sheet

Details of the supplier of the safety data sheet

Company name: AnalytiChem Services, Unipessoal, Lda
Street: Rua de Júlio Dinis 676 7º
Place: P-4050-320 Porto
Telephone: +351 226002917
E-mail: info@analytichem.com
Contact person: SDS service department
E-mail: SDS@analytichem.com
Internet: www.analytichem.com
Responsible Department: SDS service department

Supplier or manufacturer details

Company name: AnalytiChem GmbH
Street: Stempelstraße 6
Place: D-47167 Duisburg
Telephone: 0203/5194-0
E-mail: info@analytichem.de
Contact person: SDS service department
E-mail: SDS@analytichem.com
Internet: www.analytichem.de
Responsible Department: AnalytiChem:
EU-Belgium: AnalytiChem Belgium, Industriezone "De Arend" 2, 8210 Zedelgem, Belgium, +32 50 28 83 20
EU-Germany: AnalytiChem Germany, Stempelstrasse 6, 47167 Duisburg, Germany, +49 203 51 94 – 200
EU-Netherlands: AnalytiChem Netherlands, Communicatieweg 7, 3641 SG Mijdrecht, The Netherlands, +31 297 286848
UK: AnalytiChem UK, Unit 7 Launton Business Center, Murdock Road, Bicester, OX26 4XB, England, +44 1869 355 500
USA: AnalytiChem USA, 227 China Road, Winslow, Maine, 04901, United States, +1 800-244-8378
Canada: AnalytiChem Canada, 21800 Clark Graham Avenue, Baie d'Urfe, H9X 4B6, Canada, +1 514-457-0701
Australia: ORE Research & Exploration Pty Ltd, 37A Hosie Street, Bayswater North, 3153, Australia, +61 3 9729 0333
+353 1 901 4670 (CHEMTREC)

Telefax: 0203/5194-290

1.4. Emergency telephone number:

Further Information

This product is a mixture. REACH Registration Number see section 3.

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SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Regulation (EC) No 1272/2008

Eye Dam. 1; H318

Full text of hazard statements: see SECTION 16.

2.2. Label elements

Regulation (EC) No 1272/2008

Hazard components for labelling

butanol

Signal word: Danger

Pictograms:



Hazard statements

H318 Causes serious eye damage.

Precautionary statements

P280 Wear protective gloves and 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/doctor.

2.3. Other hazards

No data available

SECTION 3: Composition/information on ingredients

3.2. Mixtures

Chemical characterization

Mixtures in aqueous solution

Relevant ingredients

| CAS No | Chemical name | | | Quantity |
|-----------|--|--------------|------------------|-----------|
| | EC No | Index No | REACH No | |
| | Classification (Regulation (EC) No 1272/2008) | | | |
| 71-36-3 | butanol | | | 1 - < 5 % |
| | 200-751-6 | 603-004-00-6 | 01-2119484630-38 | |
| | Flam. Liq. 3, Acute Tox. 4, Skin Irrit. 2, Eye Dam. 1, STOT SE 3, STOT SE 3; H226 H302 H315 H318 H335 H336 | | | |
| 7647-14-5 | sodium chloride | | | 1 - < 5 % |
| | 231-598-3 | | 01-2119485491-33 | |
| | | | | |

Full text of H and EUH statements: see section 16.

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Specific Conc. Limits, M-factors and ATE

| CAS No | EC No | Chemical name | Quantity |
|-----------|-----------|--|-----------|
| | | Specific Conc. Limits, M-factors and ATE | |
| 71-36-3 | 200-751-6 | butanol | 1 - < 5 % |
| | | dermal: LD50 = ca. 3430 mg/kg; oral: LD50 = ca. 2292 mg/kg | |
| 7647-14-5 | 231-598-3 | sodium chloride | 1 - < 5 % |
| | | dermal: LD50 = > 10000 mg/kg; oral: LD50 = 3550 mg/kg | |

Further Information

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).

SECTION 4: First aid measures

4.1. Description of first aid measures

General information

No data available

After inhalation

Provide fresh air.

After contact with skin

Wash immediately with: Water

Take off immediately all contaminated clothing and wash it before reuse.

After contact with eyes

After contact with the eyes, rinse with water with the eyelids open for a sufficient length of time, then consult an ophthalmologist immediately. Remove contact lenses, if present and easy to do. Continue rinsing.

After ingestion

Rinse mouth immediately and drink plenty of water.

Call a physician immediately.

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

Irritant

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

No data available

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media

Co-ordinate fire-fighting measures to the fire surroundings.

Unsuitable extinguishing media

no restriction

5.2. Special hazards arising from the substance or mixture

Hazardous combustion products

5.3. Advice for firefighters

In case of fire: Wear self-contained breathing apparatus.

Additional information

Use water spray jet to protect personnel and to cool endangered containers.

Collect contaminated fire extinguishing water separately. Do not allow entering drains or surface water.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

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For non-emergency personnel

Provide adequate ventilation.
Use personal protection equipment.
Avoid contact with skin, eyes and clothes.
Remove persons to safety.
Emergency procedures
Consult an expert
Do not breathe dust/fume/gas/mist/vapours/spray.

For emergency responders

Precautionary statements For emergency responders : Personal protection equipment: see section 8

6.2. Environmental precautions

Do not allow to enter into surface water or drains.

6.3. Methods and material for containment and cleaning up**For containment**

Cover drains.
Prevent spread over a wide area (e.g. by containment or oil barriers).
Collect in closed and suitable containers for disposal.
Absorb with liquid-binding material (sand, diatomaceous earth, acid- or universal binding agents).

For cleaning up

Clean contaminated articles and floor according to the environmental legislation.

Other information

Provide adequate ventilation.
Do not breathe dust/fume/gas/mist/vapours/spray.
Wear breathing apparatus if exposed to vapours/dusts/aerosols.

6.4. Reference to other sections

Safe handling: see section 7
Personal protection equipment: see section 8
Disposal: see section 13

SECTION 7: Handling and storage**7.1. Precautions for safe handling****Advice on safe handling**

Handle and open container with care.
Keep container tightly closed.
Do not breathe vapour/aerosol.
Avoid contact with skin, eyes and clothes.

Advice on protection against fire and explosion

Usual measures for fire prevention.

Advice on general occupational hygiene

Wash contaminated clothing prior to re-use.
Do not breathe vapour/aerosol.
Avoid contact with skin, eyes and clothes.

Further information on handling

Wash contaminated clothing before reuse.
Wash hands before breaks and after work.

7.2. Conditions for safe storage, including any incompatibilities**Requirements for storage rooms and vessels**

Keep container tightly closed.

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Hints on joint storage

No data available

Further information on storage conditions

Store in a dry place.

7.3. Specific end use(s)

Laboratory chemicals

SECTION 8: Exposure controls/personal protection**8.1. Control parameters****Occupational exposure limits**

| CAS No | Substance | ppm | mg/m ³ | fib/cm ³ | Category | Origin |
|---------|------------|-----|-------------------|---------------------|-----------|--------|
| 71-36-3 | Butan-1-ol | 20 | - | | TWA (8 h) | |

DNEL/DMEL values

| CAS No | Substance | Exposure route | Effect | Value |
|--------------------------|-----------------|----------------|---------------------------|-------|
| 71-36-3 | butanol | | | |
| Worker DNEL, long-term | inhalation | local | 310 mg/m ³ | |
| Consumer DNEL, long-term | inhalation | systemic | 55,357 mg/m ³ | |
| Consumer DNEL, long-term | inhalation | local | 155 mg/m ³ | |
| Consumer DNEL, long-term | dermal | systemic | 3,125 mg/kg bw/day | |
| Consumer DNEL, long-term | oral | systemic | 1,562 mg/kg bw/day | |
| 7647-14-5 | sodium chloride | | | |
| Consumer DNEL, long-term | dermal | systemic | 126,65 mg/kg bw/day | |
| Consumer DNEL, acute | dermal | systemic | 126,65 mg/kg bw/day | |
| Consumer DNEL, long-term | oral | systemic | 126,65 mg/kg bw/day | |
| Consumer DNEL, acute | oral | systemic | 126,65 mg/kg bw/day | |
| Worker DNEL, long-term | inhalation | systemic | 2068,62 mg/m ³ | |
| Worker DNEL, acute | inhalation | systemic | 2068,62 mg/m ³ | |
| Worker DNEL, acute | dermal | systemic | 295,52 mg/kg bw/day | |
| Consumer DNEL, long-term | inhalation | systemic | 443,28 mg/m ³ | |
| Consumer DNEL, acute | inhalation | systemic | 443,28 mg/m ³ | |
| Worker DNEL, long-term | dermal | systemic | 295,52 mg/kg bw/day | |

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PNEC values

| CAS No | Substance | |
|--|-----------------|-------------|
| Environmental compartment | | Value |
| 71-36-3 | butanol | |
| Freshwater | | 0,082 mg/l |
| Freshwater (intermittent releases) | | 2,25 mg/l |
| Marine water | | 0,008 mg/l |
| Freshwater sediment | | 0,324 mg/kg |
| Marine sediment | | 0,032 mg/kg |
| Micro-organisms in sewage treatment plants (STP) | | 2476 mg/l |
| Soil | | 0,017 mg/kg |
| 7647-14-5 | sodium chloride | |
| Freshwater | | 5 mg/l |
| Micro-organisms in sewage treatment plants (STP) | | 500 mg/l |
| Soil | | 4,86 mg/kg |

8.2. Exposure controls

Appropriate engineering controls

Technical measures and the application of suitable work processes have priority over personal protection equipment.

Individual protection measures, such as personal protective equipment

Eye/face protection

goggles

Hand protection

Protective gloves are recommended Company KCL GmbH, D-36124 Eichenzell, email: vertrieb@kcl.de With specification (test according to EN374):

By long-term hand contact

Recommended glove articles: KCL 730 Camatril® Velours

Recommended material: NBR (Nitrile rubber) 0,4 mm

Wearing time with permanent contact: > 480 min

By short-term hand contact

Recommended glove articles: KCL 720 Camapren®

Recommended material: CR (polychloroprene, chloroprene rubber) 0,65 mm

Wearing time with occasional contact (splashes): > 120 min

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

Skin protection

Wear suitable protective clothing.

Wash hands before breaks and after work.

Respiratory protection

Respiratory protection necessary at: aerosol or mist formation

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Environmental exposure controls

Do not allow to enter into surface water or drains.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

| | | |
|---|-----------------------------|-------------------|
| Physical state: | Liquid | |
| Colour: | blue | |
| Odour: | like: aromatic hydrocarbons | |
| Odour threshold: | No data available | |
| Melting point/freezing point: | | No data available |
| Boiling point or initial boiling point and boiling range: | | No data available |
| Flammability: | | No data available |
| Lower explosion limits: | | No data available |
| Upper explosion limits: | | No data available |
| Flash point: | | No data available |
| Auto-ignition temperature: | | No data available |
| Decomposition temperature: | | No data available |
| pH-Value: | | No data available |
| Viscosity / kinematic: | | No data available |
| Water solubility: | | No data available |
| Solubility in other solvents | | |
| No data available | | |
| Partition coefficient n-octanol/water: | | No data available |
| Vapour pressure: | | No data available |
| Vapour pressure: | | No data available |
| Density: | | No data available |
| Bulk density: | | No data available |
| Relative vapour density: | | No data available |

9.2. Other information

Information with regard to physical hazard classes

| | |
|---------------------------|-------------------|
| Explosive properties | |
| No data available | |
| Sustained combustibility: | No data available |
| Self-ignition temperature | |
| Solid: | No data available |
| Gas: | No data available |
| Oxidizing properties | |
| No data available | |

Other safety characteristics

| | |
|--------------------------|-------------------|
| Evaporation rate: | No data available |
| Solvent separation test: | No data available |
| Solvent content: | No data available |
| Solid content: | 0 |
| Sublimation point: | No data available |
| Softening point: | No data available |
| Pour point: | No data available |
| No data available: | |
| Viscosity / dynamic: | No data available |
| Flow time: | No data available |

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Further Information

No data available

SECTION 10: Stability and reactivity

10.1. Reactivity

There are no data available on the mixture itself.

10.2. Chemical stability

There are no data available on the mixture itself.

10.3. Possibility of hazardous reactions

There are no data available on the mixture itself.

10.4. Conditions to avoid

There are no data available on the mixture itself.

10.5. Incompatible materials

There are no data available on the mixture itself.

10.6. Hazardous decomposition products

There are no data available on the mixture itself.

Further information

There are no data available on the mixture itself.

SECTION 11: Toxicological information

11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008**Toxicokinetics, metabolism and distribution**

There are no data available on the mixture itself.

Acute toxicity

Based on available data, the classification criteria are not met.

ATEmix calculated

ATE (oral) > 2000 mg/kg; ATE (dermal) > 2000 mg/kg; ATE (inhalation vapour) > 20 mg/l; ATE (inhalation dust/mist) > 5 mg/l

| CAS No | Chemical name | | | | |
|-----------|-----------------|---------------|----------|--------|--|
| | Exposure route | Dose | Species | Source | Method |
| 71-36-3 | butanol | | | | |
| | oral | LD50 mg/kg | ca. 2292 | Rat | Study report (1967) OECD Guideline 401 |
| | dermal | LD50 mg/kg | ca. 3430 | Rabbit | Study report (1951) OECD Guideline 402 |
| 7647-14-5 | sodium chloride | | | | |
| | oral | LD50 mg/kg | 3550 | Rat | Study report The study methodology followed appeared |
| | dermal | LD50 mg/kg | > 10000 | Rabbit | Study report The study methodology followed appeared to |

Irritation and corrosivity

Serious eye damage/eye irritation: Causes serious eye damage.

Skin corrosion/irritation: Based on available data, the classification criteria are not met.

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Sensitising effects

Based on available data, the classification criteria are not met.

Carcinogenic/mutagenic/toxic effects for reproduction

Germ cell mutagenicity: Based on available data, the classification criteria are not met.

Carcinogenicity: Based on available data, the classification criteria are not met.

Reproductive toxicity: Based on available data, the classification criteria are not met.

STOT-single exposure

Based on available data, the classification criteria are not met.

STOT-repeated exposure

Based on available data, the classification criteria are not met.

Aspiration hazard

Based on available data, the classification criteria are not met.

Specific effects in experiment on an animal

There are no data available on the mixture itself.

Additional information on tests

There are no data available on the mixture itself.

Practical experience

There are no data available on the mixture itself.

11.2. Information on other hazards**Other information**

There are no data available on the mixture itself.

Further information

There are no data available on the mixture itself.

SECTION 12: Ecological information**12.1. Toxicity**

Based on available data, the classification criteria are not met.

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| CAS No | Chemical name | | | | | |
|-----------|--------------------------|--------------|-----------|---------|------------------------------------|---|
| | Aquatic toxicity | Dose | [h] [d] | Species | Source | Method |
| 71-36-3 | butanol | | | | | |
| | Acute fish toxicity | LC50 mg/l | 1376 | 96 h | Pimephales promelas | Study report (1998) OECD Guideline 203 |
| | Acute algae toxicity | ErC50 | 225 mg/l | 96 h | Pseudokirchneriella subcapitata | Study report (1998) OECD Guideline 201 |
| | Acute crustacea toxicity | EC50 mg/l | 1328 | 48 h | Daphnia magna | Study report (1998) OECD Guideline 202 |
| | Crustacea toxicity | NOEC | 4,1 mg/l | 21 d | Daphnia magna | Study report (1996) OECD Guideline 211 |
| 7647-14-5 | sodium chloride | | | | | |
| | Acute fish toxicity | LC50 mg/l | 5840 | 96 h | Lepomis macrochirus | Study report (1985) other: ASTM E729 |
| | Acute crustacea toxicity | EC50 mg/l | 4136 | 48 h | Daphnia magna | J. fish. Res. Bd. Canada, 29: 1691-1700. OECD Guideline 202 |
| | Fish toxicity | NOEC | 252 mg/l | 33 d | Pimephales promelas | Study report (1985) OECD Guideline 210 |
| | Crustacea toxicity | NOEC | 314 mg/l | 21 d | Daphnia pulex | Memorandum of agreement No. 5429, Kentuc OECD Guideline 211 |

12.2. Persistence and degradability

There are no data available on the mixture itself.

12.3. Bioaccumulative potential

There are no data available on the mixture itself.

Partition coefficient n-octanol/water

| CAS No | Chemical name | Log Pow |
|---------|---------------|---------|
| 71-36-3 | butanol | 10 |

BCF

| CAS No | Chemical name | BCF | Species | Source |
|---------|---------------|------|---------|-------------|
| 71-36-3 | butanol | 3,16 | | QSAR (2017) |

12.4. Mobility in soil

There are no data available on the mixture itself.

12.5. Results of PBT and vPvB assessment

The substances in the mixture do not meet the PBT/vPvB criteria according to REACH, annex XIII.

12.6. Endocrine disrupting properties

This product does not contain a substance that has endocrine disrupting properties with respect to non-target organisms as no components meets the criteria.

12.7. Other adverse effects

There are no data available on the mixture itself.

Further information

Do not allow to enter into surface water or drains.

SECTION 13: Disposal considerations**13.1. Waste treatment methods**

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Disposal recommendations

Waste disposal according to directive 2008/98/EC, covering waste and dangerous waste.
Do not allow to enter into surface water or drains.

Contaminated packaging

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

SECTION 14: Transport information**Land transport (ADR/RID)**

| | |
|--|--|
| 14.1. UN number or ID number: | No dangerous good in sense of this transport regulation. |
| 14.2. UN proper shipping name: | No dangerous good in sense of this transport regulation. |
| 14.3. Transport hazard class(es): | No dangerous good in sense of this transport regulation. |
| 14.4. Packing group: | No dangerous good in sense of this transport regulation. |

Inland waterways transport (ADN)

| | |
|--|--|
| 14.1. UN number or ID number: | No dangerous good in sense of this transport regulation. |
| 14.2. UN proper shipping name: | No dangerous good in sense of this transport regulation. |
| 14.3. Transport hazard class(es): | No dangerous good in sense of this transport regulation. |
| 14.4. Packing group: | No dangerous good in sense of this transport regulation. |

Marine transport (IMDG)

| | |
|--|--|
| 14.1. UN number or ID number: | No dangerous good in sense of this transport regulation. |
| 14.2. UN proper shipping name: | No dangerous good in sense of this transport regulation. |
| 14.3. Transport hazard class(es): | No dangerous good in sense of this transport regulation. |
| 14.4. Packing group: | No dangerous good in sense of this transport regulation. |

Air transport (ICAO-TI/IATA-DGR)

| | |
|--|--|
| 14.1. UN number or ID number: | No dangerous good in sense of this transport regulation. |
| 14.2. UN proper shipping name: | No dangerous good in sense of this transport regulation. |
| 14.3. Transport hazard class(es): | No dangerous good in sense of this transport regulation. |
| 14.4. Packing group: | No dangerous good in sense of this transport regulation. |

14.5. Environmental hazards

ENVIRONMENTALLY HAZARDOUS: No

14.6. Special precautions for user

No dangerous good in sense of this transport regulation.

14.7. Maritime transport in bulk according to IMO instruments

No dangerous good in sense of this transport regulation.

SECTION 15: Regulatory information**15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture****EU regulatory information**

Restrictions on use (REACH, annex XVII):
Entry 3, Entry 40, Entry 75

National regulatory information

Water hazard class (D): 1 - slightly hazardous to water

Additional information

No data available

SECTION 16: Other information**Changes**

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This data sheet contains changes from the previous version in section(s): 2,4,5,8,9,12,15.

Abbreviations and acronyms

Flam. Liq. 3: Flammable liquids, hazard category 3

Acute Tox. 4: Acute toxicity, hazard category 4

Skin Irrit. 2: Skin irritation, hazard category 2

Eye Dam. 1: Serious eye damage, hazard category 1

STOT SE 3: Specific target organ toxicity - single exposure, hazard category 3

Classification for mixtures and used evaluation method according to Regulation (EC) No 1272/2008 [CLP]

| | |
|------------------|--------------------------|
| Classification | Classification procedure |
| Eye Dam. 1; H318 | Calculation method |

Relevant H and EUH statements (number and full text)

| | |
|------|------------------------------------|
| H226 | Flammable liquid and vapour. |
| H302 | Harmful if swallowed. |
| H315 | Causes skin irritation. |
| H318 | Causes serious eye damage. |
| H335 | May cause respiratory irritation. |
| H336 | May cause drowsiness or dizziness. |

Further Information

The above information describes exclusively the safety requirements of the product and is based on our present-day knowledge. The information is intended to give you advice about the safe handling of the product named in this safety data sheet, for storage, processing, transport and disposal. The information cannot be transferred to other products. In the case of mixing the product with other products or in the case of processing, the information on this safety data sheet is not necessarily valid for the new made-up material.

The information is based on the present level of our knowledge. It does not, however, give assurance of product properties and establishes no contract legal rights.

The receiver of our product is singularly responsible for adhering to existing laws and regulations.

Provide appropriate information, instructions and training to users

(The data for the relevant ingredients were taken respectively from the last version of the sub-contractor's safety data sheet.)