

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 04.02.2015

Version 3.2

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

1.1 Product identifier

| | |
|---------------------------|--|
| Catalogue No. | 806765 |
| Product name | 3-Nitrobenzaldehyde for synthesis |
| REACH Registration Number | A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline. |
| CAS-No. | 99-61-6 |

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

| | |
|-----------------|---|
| Identified uses | Chemical for synthesis For additional information on uses please refer to the Merck Chemicals portal (www.merckgroup.com). |
|-----------------|---|

1.3 Details of the supplier of the safety data sheet

| | |
|------------------------|---|
| Company | Merck KGaA * 64271 Darmstadt * Germany * Phone:+49 6151 72-0 |
| Responsible Department | LS-QHC * e-mail: prodsafe@merckgroup.com |

1.4 Emergency telephone number

Please contact the regional company representation in your country.

SECTION 2. Hazards identification

2.1 Classification of the substance or mixture

Classification (REGULATION (EC) No 1272/2008)

Acute toxicity, Category 4, Oral, H302

Chronic aquatic toxicity, Category 2, H411

For the full text of the H-Statements mentioned in this Section, see Section 16.

Classification (67/548/EEC or 1999/45/EC)

| | | |
|----|-------------------------------|--------|
| Xn | Harmful | R22 |
| N | Dangerous for the environment | R51/53 |

For the full text of the R-phrases mentioned in this Section, see Section 16.

2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

Hazard pictograms



Signal word
Warning

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Product name 3-Nitrobenzaldehyde for synthesis

Hazard statements

H302 Harmful if swallowed.

H411 Toxic to aquatic life with long lasting effects.

Precautionary statements

Prevention

P273 Avoid release to the environment.

Reduced labelling (≤125 ml)

Hazard pictograms



Signal word

Warning

CAS-No. 99-61-6

2.3 Other hazards

None known.

SECTION 3. Composition/information on ingredients

3.1 Substance

| | | |
|------------|---|--|
| Formula | 3-(NO ₂)C ₆ H ₄ CHO | C ₇ H ₅ NO ₃ (Hill) |
| EC-No. | 202-772-6 | |
| Molar mass | 151,12 g/mol | |

Hazardous components (REGULATION (EC) No 1272/2008)

Chemical Name (Concentration)

| CAS-No. | Registration number | Classification |
|---------|---------------------|----------------|
|---------|---------------------|----------------|

| | | |
|--------------------------------|--|--|
| 3-nitrobenzaldehyde (≤ 100 %) | | |
|--------------------------------|--|--|

| | | |
|---------|----|--|
| 99-61-6 | *) | |
|---------|----|--|

Acute toxicity, Category 4, H302

Chronic aquatic toxicity, Category 2, H411

*) A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

For the full text of the H-Statements mentioned in this Section, see Section 16.

Hazardous components (1999/45/EC)

Chemical Name (Concentration)

| CAS-No. | Classification |
|---------|----------------|
|---------|----------------|

| | |
|--------------------------------|--|
| 3-nitrobenzaldehyde (≤ 100 %) | |
|--------------------------------|--|

| | |
|---------|------------------|
| 99-61-6 | Xn, Harmful; R22 |
|---------|------------------|

N, Dangerous for the environment; R51/53

For the full text of the R-phrases mentioned in this Section, see Section 16.

3.2 Mixture

Not applicable

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SECTION 4. First aid measures

4.1 Description of first aid measures

After inhalation: fresh air.

After skin contact: wash off with plenty of water. Remove contaminated clothing.

After eye contact: rinse out with plenty of water.

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed

The following applies to aldehydes in general: irritations after contact with eyes and skin.

Mucosal irritations, coughing, and dyspnoea after inhalation.

The following applies to aromatic nitro compounds in general: systemic effect: methaemoglobinaemia with headache, cardiac dysrhythmias, drop in blood pressure, dyspnoea, and spasms; principal sign: cyanosis (blue discolouration of the blood).

4.3 Indication of any immediate medical attention and special treatment needed

No information available.

SECTION 5. Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Water, Carbon dioxide (CO₂), Foam, Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Combustible material

Development of hazardous combustion gases or vapours possible in the event of fire.

Fire may cause evolution of:

nitrogen oxides

5.3 Advice for firefighters

Special protective equipment for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

Further information

Suppress (knock down) gases/vapours/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6. Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid substance contact. Avoid inhalation of dusts. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders: Protective equipment see section 8.

6.2 Environmental precautions

Do not empty into drains.

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6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills.
Observe possible material restrictions (see sections 7 and 10).
Take up dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

6.4 Reference to other sections

Indications about waste treatment see section 13.

SECTION 7. Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Observe label precautions.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed. Dry.

Recommended storage temperature see product label.

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated.

SECTION 8. Exposure controls/personal protection

8.1 Control parameters

8.2 Exposure controls

Engineering measures

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

See section 7.1.

Individual protection measures

Protective clothing needs to be selected specifically for the workplace, depending on concentrations and quantities of the hazardous substances handled. The chemical resistance of the protective equipment should be enquired at the respective supplier.

Eye/face protection

Safety glasses

Hand protection

full contact:

| | |
|---------------------|----------------|
| Glove material: | Nitrile rubber |
| Glove thickness: | 0,11 mm |
| Break through time: | > 480 min |

splash contact:

| | |
|---------------------|----------------|
| Glove material: | Nitrile rubber |
| Glove thickness: | 0,11 mm |
| Break through time: | > 480 min |

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The protective gloves to be used must comply with the specifications of EC Directive 89/686/EEC and the related standard EN374, for example KCL 741 Dermatril® L (full contact), KCL 741 Dermatril® L (splash contact).

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).

Respiratory protection

required when dusts are generated.

Recommended Filter type: Filter P 2 (acc. to DIN 3181) for solid and liquid particles of harmful substances

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Environmental exposure controls

Do not empty into drains.

SECTION 9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

| | |
|-----------------------------|---------------------------|
| Form | powder, finecrystalline |
| Colour | yellow |
| Odour | bitter almond-like |
| Odour Threshold | No information available. |
| pH | No information available. |
| Melting point | 54 - 57 °C |
| Boiling point/boiling range | 164 °C at 31 hPa |
| Flash point | No information available. |
| Evaporation rate | No information available. |
| Flammability (solid, gas) | No information available. |
| Lower explosion limit | No information available. |
| Upper explosion limit | No information available. |
| Vapour pressure | No information available. |
| Relative vapour density | No information available. |

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| | |
|---------------|-----------------------------------|
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| | |
|--|--|
| Density | No information available. |
| Relative density | No information available. |
| Water solubility | 1,6 g/l at 25 °C |
| Partition coefficient: n-octanol/water | log Pow: 1,47 (experimental) (Lit.) Bioaccumulation is not expected. |
| Auto-ignition temperature | No information available. |
| Decomposition temperature | No information available. |
| Viscosity, dynamic | No information available. |
| Explosive properties | No information available. |
| Oxidizing properties | No information available. |

9.2 Other data

none

SECTION 10. Stability and reactivity

10.1 Reactivity

The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidizing agents, Strong bases

10.4 Conditions to avoid

Strong heating.

10.5 Incompatible materials

no information available

10.6 Hazardous decomposition products

in the event of fire: See section 5.

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SECTION 11. Toxicological information

11.1 Information on toxicological effects

Acute oral toxicity

LD50 Rat: 1.075 mg/kg (External MSDS)

Symptoms: We have no description of any toxic symptoms.
absorption

Acute inhalation toxicity

This information is not available.

Acute dermal toxicity

This information is not available.

Skin irritation

This information is not available.

Eye irritation

This information is not available.

Sensitisation

This information is not available.

Germ cell mutagenicity

This information is not available.

Carcinogenicity

This information is not available.

Reproductive toxicity

This information is not available.

Teratogenicity

This information is not available.

Specific target organ toxicity - single exposure

This information is not available.

Specific target organ toxicity - repeated exposure

This information is not available.

Aspiration hazard

This information is not available.

11.2 Further information

The following applies to aldehydes in general: irritations after contact with eyes and skin.

Mucosal irritations, coughing, and dyspnoea after inhalation.

The following applies to aromatic nitro compounds in general: systemic effect:

methaemoglobinaemia with headache, cardiac dysrhythmias, drop in blood pressure, dyspnoea, and spasms; principal sign: cyanosis (blue discolouration of the blood).

Further data:

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

12.1 Toxicity

Toxicity to fish

LC50 Pimephales promelas (fathead minnow): 5,8 mg/l; 96 h (ECOTOX Database)

12.2 Persistence and degradability

No information available.

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12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 1,47

(experimental)

(Lit.) Bioaccumulation is not expected.

12.4 Mobility in soil

No information available.

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted.

12.6 Other adverse effects

Additional ecological information

Discharge into the environment must be avoided.

SECTION 13. Disposal considerations

Waste treatment methods

See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14. Transport information

Land transport (ADR/RID)

14.1 UN number UN 3077

14.2 Proper shipping name ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (3-NITROBENZALDEHYDE)

14.3 Class 9

14.4 Packing group III

14.5 Environmentally hazardous yes

14.6 Special precautions for user yes

Tunnel restriction code E

Packages smaller than or equal to 5 kg / L , not dangerous goods of Class 9

Inland waterway transport (ADN)

Not relevant

Air transport (IATA)

14.1 UN number UN 3077

14.2 Proper shipping name ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (3-NITROBENZALDEHYDE)

14.3 Class 9

14.4 Packing group III

14.5 Environmentally hazardous yes

14.6 Special precautions for user no

Packages smaller than or equal to 5 kg / L , not dangerous goods of Class 9

Sea transport (IMDG)

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Product name 3-Nitrobenzaldehyde for synthesis

14.1 UN number UN 3077
14.2 Proper shipping name ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (3-NITROBENZALDEHYDE)
14.3 Class 9
14.4 Packing group III
14.5 Environmentally hazardous yes
14.6 Special precautions for user yes
EmS F-A S-F
Packages smaller than or equal to 5 kg / L , not dangerous goods of Class 9
14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code
Not relevant

SECTION 15. Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

EU regulations

Major Accident Hazard 96/82/EC
Legislation Dangerous for the environment
9b
Quantity 1: 200 t
Quantity 2: 500 t

Occupational restrictions Take note of Dir 94/33/EC on the protection of young people at work. Take note of Dir 92/85/EEC on the safety and health at work of pregnant workers.

Regulation (EC) No 1005/2009 on substances that deplete the ozone layer not regulated

Regulation (EC) No 850/2004 of the European Parliament and of the Council of 29 April 2004 on persistent organic pollutants and amending Directive 79/117/EEC not regulated

Regulation (EC) No 689/2008 concerning the export and import of dangerous chemicals not regulated

Substances of very high concern (SVHC) 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 $\geq 0.1\%$ (w/w).

National legislation

Storage class 10 - 13

15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out.

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SECTION 16. Other information

Full text of H-Statements referred to under sections 2 and 3.

H302 Harmful if swallowed.
H411 Toxic to aquatic life with long lasting effects.

Full text of R-phrases referred to under sections 2 and 3

R22 Harmful if swallowed.
R51/53 Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

Training advice

Provide adequate information, instruction and training for operators.

Labelling

Hazard pictograms



Signal word

Warning



Hazard statements

H302 Harmful if swallowed.
H411 Toxic to aquatic life with long lasting effects.

Precautionary statements

Prevention
P273 Avoid release to the environment.

Labelling (67/548/EEC or 1999/45/EC)

| | | |
|-----------|--|---|
| Symbol(s) |  Xn | Harmful |
| |  N | Dangerous for the environment |
| R-phrases | 22-51/53 | Harmful if swallowed. Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment. |
| S-phrases | 61 | Avoid release to the environment. Refer to special instructions/ Safety data sheets. |
| EC-No. | 202-772-6 | |

Reduced labelling (≤125 ml)

| | | |
|-----------|--|-------------------------------|
| Symbol(s) |  Xn | Harmful |
| |  N | Dangerous for the environment |
| R-phrases | 22 | Harmful if swallowed. |

Key or legend to abbreviations and acronyms used in the safety data sheet

Used abbreviations and acronyms can be looked up at www.wikipedia.org.

Regional representation

This information is given on the authorised Safety Data Sheet for your country.

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| | |
|---------------|-----------------------------------|
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The information contained herein is based on the present state of our knowledge. It characterises the product with regard to the appropriate safety precautions. It does not represent a guarantee of any properties of the product.