

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 16.12.2010

Version 6.4

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

### 1.1 Product identifier

|                           |  |
|---------------------------|--|
| Catalogue No.             | 803120   |
| Product name              | 1,4-Dinitrobenzene 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. |

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

|                 |   |
|-----------------|---|
| Identified uses | Chemical for synthesis<br>For additional information on uses please refer to the Merck Chemicals portal ( <a href="http://www.merck-chemicals.com">www.merck-chemicals.com</a> ). |
|-----------------|---|

### 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: <a href="mailto:prodsafe@merckgroup.com">prodsafe@merckgroup.com</a> |

### 1.4 Emergency telephone number

Please contact the regional company representation in your country.

## 2. Hazards identification

### 2.1 Classification of the substance or mixture

#### Classification (REGULATION (EC) No 1272/2008)

Acute toxicity, Category 2, Inhalation, H330  
 Acute toxicity, Category 1, Dermal, H310  
 Acute toxicity, Category 2, Oral, H300  
 Specific target organ toxicity - repeated exposure, Category 2, H373  
 Acute aquatic toxicity, Category 1, H400  
 Chronic aquatic toxicity, Category 1, H410

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

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

|    |                               |                  |
|----|-------------------------------|------------------|
| T+ | Very toxic                    | R26/27/28<br>R33 |
| N  | Dangerous for the environment | R50/53           |

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



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*Signal word*

Danger

*Hazard statements*

H300 + H310 + H330 Fatal if swallowed, in contact with skin or if inhaled.  
H373 May cause damage to organs through prolonged or repeated exposure.  
H410 Very toxic to aquatic life with long lasting effects.

*Precautionary statements*

P273 Avoid release to the environment.  
P280 Wear protective gloves/ protective clothing.  
P302 + P352 IF ON SKIN: Wash with plenty of soap and water.  
P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.  
P309 + P310 IF exposed or if you feel unwell: Immediately call a POISON CENTER or doctor/physician.

**Reduced labelling (≤125 ml)**

*Hazard pictograms*



*Signal word*

Danger

*Hazard statements*

H300 + H310 + H330 Fatal if swallowed, in contact with skin or if inhaled.

*Precautionary statements*

P280 Wear protective gloves/ protective clothing.

*Index-No.* 609-004-00-2

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

|              |                   |   |
|--------------|-------------------|---|
| Symbol(s)    | T+<br>N           | Very toxic<br>Dangerous for the environment   |
| R-phrases(s) | 26/27/28-33-50/53 | Very toxic by inhalation, in contact with skin and if swallowed.<br>Danger of cumulative effects. Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.  |
| S-phrases(s) | 28-36/37-45-60-61 | After contact with skin, wash immediately with plenty of soap and water. Wear suitable protective clothing and gloves. In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible). This material and its container must be disposed of as hazardous waste. Avoid release to the environment. Refer to special instructions/ Safety data sheets. |

EC-No. 202-833-7 EC Label

**Reduced labelling (≤125 ml)**

|              |             |  |
|--------------|-------------|--|
| Symbol(s)    | T+<br>N     | Very toxic<br>Dangerous for the environment  |
| R-phrases(s) | 26/27/28    | Very toxic by inhalation, in contact with skin and if swallowed.   |
| S-phrases(s) | 28-36/37-45 | After contact with skin, wash immediately with plenty of soap and water. Wear suitable protective clothing and gloves. In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible). |

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### 2.3 Other hazards

None known.

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### 3. Composition/information on ingredients

|            |   |  |
|------------|---|--|
| Formula    | 1,4-(NO <sub>2</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>4</sub> | C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> O <sub>4</sub> (Hill) |
| CAS-No.    | 100-25-4  |  |
| Index-No.  | 609-004-00-2  |  |
| EC-No.     | 202-833-7   |  |
| Molar mass | 168,1 g/mol   |  |

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### 4. First aid measures

#### 4.1 Description of first aid measures

##### *General advice*

First aider needs to protect himself.

After inhalation: fresh air. If breathing stops: immediately apply artificial respiration, if necessary oxygen. Immediately call in physician.

After skin contact: wash off with plenty of water. Swab with polyethylene glycol 400. Immediately remove contaminated clothing. Call a physician immediately.

After eye contact: rinse out with plenty of water.

If swallowed: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only in persons who are wide awake and fully conscious), administer activated charcoal (20 - 40 g in a 10% slurry) and consult a doctor as quickly as possible.

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

irritant effects, Cough, Shortness of breath, Dizziness, Nausea, Vomiting, confusion, Coma

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 immediate medical attention and special treatment needed

No information available.

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### 5. Fire-fighting measures

#### 5.1 Extinguishing media

##### *Suitable extinguishing media*

Carbon dioxide (CO<sub>2</sub>), Foam, Dry powder, Water

##### *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

Explosive decomposition possible on heating.

Forms explosive mixtures with air on intense heating.

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

Fire may cause evolution of:

nitrogen oxides, nitrous gases

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### 5.3 Advice for firefighters

*Special protective equipment for fire-fighters*

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.

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## 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.

### 6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills.

Observe possible material restrictions (see sections 7.2 and 10.5).

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.

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## 7. Handling and storage

### 7.1 Precautions for safe handling

Observe label precautions.

Work under hood. Do not inhale substance.

### 7.2 Conditions for safe storage, including any incompatibilities

Dry. Tightly closed. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorised persons.

Store at +15°C to +25°C.

### 7.3 Specific end uses

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

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## 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.

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**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.

*Hygiene measures*

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

*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      |

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](http://www.kcl.de)).

*Other protective equipment*

protective clothing

*Respiratory protection*

required

Recommended Filter type: Filter A-(P3)

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.

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**9. Physical and chemical properties**

**9.1 Information on basic physical and chemical properties**

|                 |                           |
|-----------------|---------------------------|
| Form            | powder, finocrystalline   |
| Colour          | beige                     |
| Odour           | No information available. |
| Odour Threshold | No information available. |

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|  |  |
|--|--|
| pH                                     | No information available.  |
| Melting point                          | 174 °C   |
| Boiling point/boiling range            | 299 °C<br>at 1.013 hPa   |
| Flash point                            | 150 °C   |
| 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.  |
| Relative density                       | No information available.  |
| Water solubility                       | 0,069 g/l<br>at 25 °C  |
| Partition coefficient: n-octanol/water | log Pow: 1,46<br>Method: (experimental)<br>Bioaccumulation is not expected. (Lit.) |
| Autoignition 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

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**10. Stability and reactivity**

**10.1 Reactivity**

sensitive to shock

steam-volatile

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

Forms explosive mixtures with air on intense heating.

**10.2 Chemical stability**

heat-sensitive

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**10.3 Possibility of hazardous reactions**

Risk of explosion with:

Ammonia, bases, Nitric acid, Reducing agents, chlorates, Potassium hydroxide, Alkali metals  
aluminium chloride, with, phenol

Exothermic reaction with:

Fluorine, sodium, Oxidizing agents, Strong bases

**10.4 Conditions to avoid**

Avoid shock and friction.

Heating.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

**10.5 Incompatible materials**

no information available

**10.6 Hazardous decomposition products**

in the event of fire: See chapter 5.

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**11. Toxicological information**

**11.1 Information on toxicological effects**

*Acute oral toxicity*

Symptoms: Nausea, Vomiting

absorption

*Acute inhalation toxicity*

Rapid absorption.

*Acute dermal toxicity*

Rapid absorption.

*Skin irritation*

Irritations

*Eye irritation*

Irritations

*Specific target organ toxicity - single exposure*

The substance or mixture is not classified as specific target organ toxicant, single exposure.

*Specific target organ toxicity - repeated exposure*

May cause damage to organs through prolonged or repeated exposure.

*Aspiration hazard*

Based on available data the classification criteria are not met.

**11.2 Further information**

*Further information*

Quantitative data on the toxicity of this product are not available.

Further toxicological data:

Systemic effects:

After absorption:

After a latency period:

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Methaemoglobinaemia with headache, cardiac arrhythmia, drop in blood pressure, dyspnoea, and spasms; key symptom: cyanosis (blue colouration of the blood).

Dizziness, confusion, Nausea, Vomiting, Coma

Effect potentiated by: ethanol

Chronic intoxication:

Damage to:

Liver

Danger of cumulative effects.

Other information

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.

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## 12. Ecological information

### 12.1 Toxicity

*Toxicity to fish*

LC50

Species: *Ictalurus catus* (catfish)

Dose: 0,673 mg/l

Exposure time: 96 h

(above the solubility limit in the test medium) (ECOTOX Database)

### 12.2 Persistence and degradability

No information available.

### 12.3 Bioaccumulative potential

*Partition coefficient: n-octanol/water*

log Pow: 1,46

Method: (experimental)

Bioaccumulation is not expected. (Lit.)

### 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*

Do not allow to run into surface waters, wastewater, or soil.



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### 13. Disposal considerations

*Waste treatment methods*

See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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### 14. Transport information

**ADR/RID**

UN 3443 DINITROBENZENES, SOLID, 6.1, II

**IATA**

UN 3443 DINITROBENZENES, SOLID, 6.1, II

**IMDG**

UN 3443 DINITROBENZENES, SOLID, 6.1, II

EmS F-A S-A

The transport regulations are cited according to international regulations and in the form applicable in Germany. Possible national deviations in other countries are not considered.

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### 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 Very toxic  
1  
Quantity 1: 5 t  
Quantity 2: 20 t

96/82/EC  
Dangerous for the environment  
9a  
Quantity 1: 100 t  
Quantity 2: 200 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.

*National legislation*

Storage class VCI 6.1A Combustible substances, toxic

#### 15.2 Chemical Safety Assessment

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

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### 16. Other information

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

H300 Fatal if swallowed.  
H310 Fatal in contact with skin.  
H330 Fatal if inhaled.  
H373 May cause damage to organs through prolonged or repeated

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H400 exposure.  
Very toxic to aquatic life.  
H410 Very toxic to aquatic life with long lasting effects.

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

R26/27/28 Very toxic by inhalation, in contact with skin and if swallowed.  
R33 Danger of cumulative effects.  
R50/53 Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

**Training advice**

Provide adequate information, instruction and training for operators.

**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](http://www.wikipedia.org).

**Regional representation**

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

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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.*