

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name : 1-Chloro-4-nitrobenzene

Product Number : C59122

Brand : Aldrich

Index-No. : 610-005-00-5

CAS-No. : 100-00-5

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

Identified uses : Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA

Telephone : +1 800-325-5832

Fax : +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Acute toxicity, Oral (Category 3), H301

Acute toxicity, Inhalation (Category 3), H331

Acute toxicity, Dermal (Category 3), H311

Germ cell mutagenicity (Category 2), H341

Carcinogenicity (Category 2), H351

Specific target organ toxicity - repeated exposure (Category 2), H373

Acute aquatic toxicity (Category 2), H401

Chronic aquatic toxicity (Category 2), H411

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

2.2 GHS Label elements, including precautionary statements

Pictogram



Signal word

Danger

Hazard statement(s)

H301 + H311 + H331
H341
H351
H373
H411

Toxic if swallowed, in contact with skin or if inhaled.

Suspected of causing genetic defects.

Suspected of causing cancer.

May cause damage to organs through prolonged or repeated exposure.

Toxic to aquatic life with long lasting effects.

| | |
|----------------------------|--|
| Precautionary statement(s) | |
| P201 | Obtain special instructions before use. |
| P202 | Do not handle until all safety precautions have been read and understood. |
| P260 | Do not breathe dust/ fume/ gas/ mist/ vapours/ spray. |
| P264 | Wash skin thoroughly after handling. |
| P270 | Do not eat, drink or smoke when using this product. |
| P271 | Use only outdoors or in a well-ventilated area. |
| P273 | Avoid release to the environment. |
| P280 | Wear protective gloves/ protective clothing. |
| P301 + P310 | IF SWALLOWED: Immediately call a POISON CENTER/doctor. |
| 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. |
| P308 + P313 | IF exposed or concerned: Get medical advice/ attention. |
| P322 | Specific measures (see supplemental first aid instructions on this label). |
| P330 | Rinse mouth. |
| P361 | Remove/Take off immediately all contaminated clothing. |
| P363 | Wash contaminated clothing before reuse. |
| P391 | Collect spillage. |
| P403 + P233 | Store in a well-ventilated place. Keep container tightly closed. |
| P405 | Store locked up. |
| P501 | Dispose of contents/ container to an approved waste disposal plant. |

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

| | | |
|------------------|---|---|
| Formula | : | C ₆ H ₄ ClNO ₂ |
| Molecular weight | : | 157.55 g/mol |
| CAS-No. | : | 100-00-5 |
| EC-No. | : | 202-809-6 |
| Index-No. | : | 610-005-00-5 |

Hazardous components

| Component | Classification | Concentration |
|--------------------------------|---|---------------|
| 1-Chloro-4-nitrobenzene | Acute Tox. 3; Muta. 2; Carc. 2; STOT RE 2; Aquatic Acute 2; Aquatic Chronic 2; H301 + H311 + H331, H341, H351, H373, H411 | 90 - 100 % |

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

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

In case of eye contact

Flush eyes with water as a precaution.

If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

5. FIREFIGHTING MEASURES**5.1 Extinguishing media****Suitable extinguishing media**

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

5.2 Special hazards arising from the substance or mixture

No data available

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

No data available

6. ACCIDENTAL RELEASE MEASURES**6.1 Personal precautions, protective equipment and emergency procedures**

Wear respiratory protection. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust. For personal protection see section 8.

6.2 Environmental precautions

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

6.3 Methods and materials for containment and cleaning up

Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

6.4 Reference to other sections

For disposal see section 13.

7. HANDLING AND STORAGE**7.1 Precautions for safe handling**

Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Provide appropriate exhaust ventilation at places where dust is formed. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Storage class (TRGS 510): 6.1B: Non-combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials

7.3 Specific end use(s)

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

8. EXPOSURE CONTROLS/PERSONAL PROTECTION**8.1 Control parameters****Components with workplace control parameters**

| Component | CAS-No. | Value | Control parameters | Basis |
|-----------|---------|--|--------------------|-------|
| | Remarks | Potential Occupational Carcinogen See Appendix A Potential for dermal absorption | | |

| | | | | |
|-------------------------|----------|---|-----------------------|---|
| 1-Chloro-4-nitrobenzene | 100-00-5 | TWA | 0.1 ppm | USA. ACGIH Threshold Limit Values (TLV) |
| | | Methemoglobinemia Substances for which there is a Biological Exposure Index or Indices (see BEI® section), see BEI® for Methemoglobin Inducers Confirmed animal carcinogen with unknown relevance to humans Danger of cutaneous absorption | | |
| | | TWA | 0.100000 ppm | USA. ACGIH Threshold Limit Values (TLV) |
| | | Methemoglobinemia Substances for which there is a Biological Exposure Index or Indices (see BEI® section), see BEI® for Methemoglobin Inducers Confirmed animal carcinogen with unknown relevance to humans Danger of cutaneous absorption | | |
| | | TWA | 1.000000 mg/m3 | USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants |
| | | Skin designation | | |
| | | PEL | 0.1 ppm 0.64 mg/m3 | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |
| | | Skin | | |

8.2 Exposure controls

Appropriate engineering controls

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

Personal protective equipment

Eye/face protection

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: Dermatrill® (KCL 740 / Aldrich Z677272, Size M)

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: Dermatrill® (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face particle respirator type N100 (US) or type P3 (EN 143) respirator cartridges as a backup to engineering controls. If the respirator is the

sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

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

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

| | |
|---|--|
| a) Appearance | Form: crystalline Colour: light yellow |
| b) Odour | No data available |
| c) Odour Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | Melting point/range: 83 - 84 °C (181 - 183 °F) |
| f) Initial boiling point and boiling range | 242 °C (468 °F) at 1,013 hPa (760 mmHg) |
| g) Flash point | 124 °C (255 °F) - closed cup |
| h) Evaporation rate | No data available |
| i) Flammability (solid, gas) | No data available |
| j) Upper/lower flammability or explosive limits | No data available |
| k) Vapour pressure | No data available |
| l) Vapour density | No data available |
| m) Relative density | 1.298 g/cm ³ |
| n) Water solubility | insoluble |
| o) Partition coefficient: n-octanol/water | log Pow: 2.6 |
| p) Auto-ignition temperature | No data available |
| q) Decomposition temperature | No data available |
| r) Viscosity | No data available |
| s) Explosive properties | No data available |
| t) Oxidizing properties | No data available |

9.2 Other safety information

No data available

10. STABILITY AND REACTIVITY

10.1 Reactivity

No data available

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

No data available

10.5 Incompatible materials

Strong oxidizing agents, Strong bases

10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NOx), Hydrogen chloride gas

Other decomposition products - No data available

In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - 420 mg/kg

Remarks: Behavioral:Somnolence (general depressed activity). Liver:Fatty liver degeneration.

Blood:Methemoglobinemia-Carboxyhemoglobin.

No data available

Skin corrosion/irritation

Skin - Rabbit

Result: Mild skin irritation

Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation

Respiratory or skin sensitisation

No data available

Germ cell mutagenicity

Laboratory experiments have shown mutagenic effects.

In vitro tests showed mutagenic effects

Carcinogenicity

This product is or contains a component that is not classifiable as to its carcinogenicity based on its IARC, ACGIH, NTP, or EPA classification.

Limited evidence of carcinogenicity in animal studies

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity

No data available

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

May cause damage to organs through prolonged or repeated exposure.

Aspiration hazard

No data available

Additional Information

RTECS: Not available

May cause cyanosis.

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to daphnia and other aquatic invertebrates EC50 - Daphnia magna (Water flea) - 2.7 mg/l - 48 h

Toxicity to algae Growth inhibition EC50 - Chlorella pyrenoidosa - 4.9 mg/l - 96 h

12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 28 d

12.3 Bioaccumulative potential

Bioaccumulation Oncorhynchus mykiss (rainbow trout) - 36 d
- 0.780 µg/l

Bioconcentration factor (BCF): 108

12.4 Mobility in soil

No data 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

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.
Toxic to aquatic life with long lasting effects.

No data available

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

Contaminated packaging

Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)

UN number: 1578 Class: 6.1 Packing group: II
Proper shipping name: Chloronitrobenzenes, solid

Poison Inhalation Hazard: No

IMDG

UN number: 1578 Class: 6.1 Packing group: II EMS-No: F-A, S-A
Proper shipping name: CHLORONITROBENZENES, SOLID
Marine pollutant: yes

IATA

UN number: 1578 Class: 6.1 Packing group: II
Proper shipping name: Chloronitrobenzenes, solid

15. REGULATORY INFORMATION

SARA 302 Components

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards

Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

| | | |
|-------------------------|---------------------|-----------------------------|
| 1-Chloro-4-nitrobenzene | CAS-No. 100-00-5 | Revision Date 1993-04-24 |
|-------------------------|---------------------|-----------------------------|

| | | |
|-------------------------|---------------------|-----------------------------|
| 1-Chloro-4-nitrobenzene | CAS-No. 100-00-5 | Revision Date 1993-04-24 |
|-------------------------|---------------------|-----------------------------|

Pennsylvania Right To Know Components

| | | |
|-------------------------|---------------------|-----------------------------|
| 1-Chloro-4-nitrobenzene | CAS-No. 100-00-5 | Revision Date 1993-04-24 |
|-------------------------|---------------------|-----------------------------|

| | | |
|-------------------------|---------------------|-----------------------------|
| 1-Chloro-4-nitrobenzene | CAS-No. 100-00-5 | Revision Date 1993-04-24 |
|-------------------------|---------------------|-----------------------------|

| | | |
|-------------------------|---------------------|-----------------------------|
| 1-Chloro-4-nitrobenzene | CAS-No. 100-00-5 | Revision Date 1993-04-24 |
|-------------------------|---------------------|-----------------------------|

New Jersey Right To Know Components

| | | |
|-------------------------|---------------------|-----------------------------|
| 1-Chloro-4-nitrobenzene | CAS-No. 100-00-5 | Revision Date 1993-04-24 |
|-------------------------|---------------------|-----------------------------|

| | | |
|-------------------------|---------------------|-----------------------------|
| 1-Chloro-4-nitrobenzene | CAS-No. 100-00-5 | Revision Date 1993-04-24 |
|-------------------------|---------------------|-----------------------------|

California Prop. 65 Components

| | | |
|---|---------------------|-----------------------------|
| WARNING! This product contains a chemical known to the State of California to cause cancer. | CAS-No. 100-00-5 | Revision Date 2007-09-28 |
| 1-Chloro-4-nitrobenzene | | |

16. OTHER INFORMATION

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

| | |
|--------------------|---|
| Acute Tox. | Acute toxicity |
| Aquatic Acute | Acute aquatic toxicity |
| Aquatic Chronic | Chronic aquatic toxicity |
| Carc. | Carcinogenicity |
| H301 | Toxic if swallowed. |
| H301 + H311 + H331 | Toxic if swallowed, in contact with skin or if inhaled. |
| H311 | Toxic in contact with skin. |
| H331 | Toxic if inhaled. |
| H341 | Suspected of causing genetic defects. |
| H351 | Suspected of causing cancer. |

HMIS Rating

| | |
|------------------------|---|
| Health hazard: | 2 |
| Chronic Health Hazard: | * |
| Flammability: | 1 |
| Physical Hazard | 0 |

NFPA Rating

| | |
|--------------------|---|
| Health hazard: | 2 |
| Fire Hazard: | 1 |
| Reactivity Hazard: | 0 |

Further information

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Preparation Information

Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

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