



MATERIAL SAFETY DATA SHEET

according to the Global Harmonized System

Date of issue: 02/04/2013

Version 1.0

SECTION 1. Identification

Product identifier

Product number 820446
Product name 1,3-Dichloro-4-nitrobenzene for synthesis

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

Identified uses Chemical for synthesis

Details of the supplier of the safety data sheet

Company EMD Millipore Corporation | 290 Concord Road, Billerica, MA 01821,
United States of America | SDS Phone Support: +1-978-715-1335 |
General Inquiries: +1-978-751-4321 | Monday to Friday, 9:00 AM to
4:00 PM Eastern Time (GMT-5)

e-mail: mm_sds@merckgroup.com

Emergency telephone 613-996-6666 CANUTEC (Canada)
+1-703-527-3887 CHEMTREC (International)
24 Hours/day; 7 Days/week

SECTION 2. Hazards identification

GHS Classification

Acute toxicity, Category 3, Dermal, H311
Acute toxicity, Category 4, Oral, H302
Skin sensitization, Category 1, H317
Chronic aquatic toxicity, Category 2, H411

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

GHS-Labeling

Hazard pictograms



Signal Word
Danger

Hazard Statements
H302 Harmful if swallowed.

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H311 Toxic in contact with skin.
H317 May cause an allergic skin reaction.
H411 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.
P309 + P310 IF exposed or if you feel unwell: Immediately call a POISON CENTER or doctor/physician.

Other hazards

None known.

SECTION 3. Composition/information on ingredients

Formula	1,3-(Cl) ₂ C ₆ H ₃ -4-(NO ₂)	C ₆ H ₃ Cl ₂ NO ₂ (Hill)
CAS-No.	611-06-3	
Molar mass	192 g/mol	

Hazardous ingredients

Chemical Name (Concentration)

CAS-No.
1,3-Dichloro-4-nitrobenzene (>= 90 % - <= 100 %)
611-06-3

SECTION 4. First aid measures

Description of first-aid measures

Inhalation

After inhalation: fresh air.

Skin contact

After skin contact: wash off with plenty of water. Remove contaminated clothing. Call a physician immediately.

Eye contact

After eye contact: rinse out with plenty of water.

Ingestion

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

Never give anything by mouth to an unconscious person.

Most important symptoms and effects, both acute and delayed

Allergic reactions

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

Indication of any immediate medical attention and special treatment needed

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No information available.

SECTION 5. Fire-fighting measures

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.

Special hazards arising from the substance or mixture

Combustible material

Risk of dust explosion.

Forms explosive mixtures with air on intense heating.

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

Fire may cause evolution of:

Hydrogen chloride gas, nitrogen oxides

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

Prevent fire extinguishing water from contaminating surface water or the ground water system.

Suppress (knock down) gases/vapors/mists with a water spray jet.

SECTION 6. Accidental release measures

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.

Environmental precautions

Do not empty into drains.

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.

SECTION 7. Handling and storage

Precautions for safe handling

Observe label precautions.

Conditions for safe storage, including any incompatibilities

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

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Store at +15°C to +25°C (+59°F to +77°F).

SECTION 8. Exposure controls/personal protection

Exposure limit(s)

Contains no substances with occupational exposure limit values.

Engineering measures

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

Individual protection measures

Protective clothing should be selected specifically for the workplace, depending on concentration and quantity of the hazardous substances handled. The chemical resistance of the protective equipment should be inquired at the respective supplier.

Hygiene measures

Immediately change contaminated clothing. Apply skin- protective barrier cream. Wash hands and face after working with substance. Work under hood. Do not inhale substance/mixture.

Eye/face protection

Safety glasses

Hand protection

Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

Other protective equipment:

protective clothing

Respiratory protection

required when dusts are generated.

Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

SECTION 9. Physical and chemical properties

Physical state	crystals
Color	yellow
Odor	weakly aromatic
Odor Threshold	No information available.
pH	No information available.
Melting point	28 - 31 °C
Boiling point/boiling range	498 °F (259 °C)
Flash point	306 °F (152 °C)
Evaporation rate	No information available.

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Flammability (solid, gas)	No information available.
Lower explosion limit	No information available.
Upper explosion limit	No information available.
Vapor pressure	0.013 hPa at 68 °F (20 °C)
Relative vapor density	6.63
Relative density	1.51 g/cm ³
Water solubility	188 g/l at 68 °F (20 °C)
Partition coefficient: n-octanol/water	log Pow: 3.07 (experimental) (Lit.) Bioaccumulation is not expected (log Pow <1).
Autoignition temperature	No information available.
Decomposition temperature	> 662 °F (> 350 °C)
Viscosity, dynamic	No information available.
Explosive properties	No information available.
Ignition temperature	932 °F (500 °C)

SECTION 10. Stability and reactivity

Reactivity

Forms explosive mixtures with air on intense heating.
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.

Chemical stability

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

Possibility of hazardous reactions

Violent reactions possible with:
bases, Strong oxidizing agents, strong alkalis

Conditions to avoid

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

Incompatible materials

no information available

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Hazardous decomposition products
in the event of fire: See section 5.

SECTION 11. Toxicological information

Information on toxicological effects

Likely route of exposure

Eye contact, Skin contact, Ingestion

Acute oral toxicity

LD50 rat: 380 mg/kg (External MSDS)

Symptoms: We have no description of any toxic symptoms.

Acute dermal toxicity

LD50 rat: 920 mg/kg

(External MSDS)

Symptoms: We have no description of any toxic symptoms.

Sensitization

May cause sensitization by skin contact.

May cause an allergic skin reaction.

Genotoxicity in vitro

Mutagenicity (mammal cell test): chromosome aberration.

Result: negative

(National Toxicology Program)

Ames test

Salmonella typhimurium

Result: positive

(National Toxicology Program)

Specific target organ systemic toxicity - single exposure

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

Specific target organ systemic toxicity - repeated exposure

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

Aspiration hazard

Regarding the available data the classification criteria are not fulfilled.

Carcinogenicity

IARC	No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.
OSHA	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.
NTP	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.
ACGIH	No ingredient of this product present at levels greater than or

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equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

Further information

Other information

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

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

Ecotoxicity

Toxicity to daphnia and other aquatic invertebrates

EC50 Daphnia magna (Water flea): 4.2 mg/l; 48 h (ECOTOX Database)

Toxicity to algae

IC50 chlorella pyrenoidosa: 2.4 mg/l; 96 h (ECOTOX Database)

Persistence and degradability

No information available.

Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 3.07

(experimental)

(Lit.) Bioaccumulation is not expected (log Pow <1).

Mobility in soil

No information available.

Other adverse effects

Additional ecological information

Discharge into the environment must be avoided.

SECTION 13. Disposal considerations

The information presented only applies to the material as supplied. The identification based on characteristic(s) or listing may not apply if the material has been used or otherwise contaminated. It is the responsibility of the waste generator to determine the toxicity and physical properties of the material generated to determine the proper waste identification and disposal methods in compliance with applicable regulations. Disposal should be in accordance with applicable regional, national and local laws and regulations.

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SECTION 14. Transport information

Land transport (DOT)

UN number UN 3077
Proper shipping name ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID,
N.O.S. (1,3-DICHLORO-4-NITROBENZENE)
Class 9
Packing group III
Environmentally hazardous --

Air transport (IATA)

UN number UN 3077
Proper shipping name ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID,
N.O.S. (1,3-DICHLORO-4-NITROBENZENE)
Class 9
Packing group III
Environmentally hazardous --
Special precautions for user no

Sea transport (IMDG)

UN number UN 3077
Proper shipping name ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID,
N.O.S. (1,3-DICHLORO-4-NITROBENZENE)
Class 9
Packing group III
Environmentally hazardous --
Special precautions for user yes
EmS F-A S-F

SECTION 15. Regulatory information

United States of America

Canada

WHMIS Classification

D1B Toxic Material Causing Immediate and Serious Toxic Effects

D2B Toxic Material Causing Other Toxic Effects

Toxic by ingestion, Toxic by skin absorption, Skin sensitizer

This product has been classified according to the hazard criteria of the CPR and the MSDS contains all of the information required by the CPR.

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Notification status

TSCA: On TSCA Inventory

DSL: This product contains one or several components listed in the
Canadian NDSL.
Ingredients
1,3-Dichloro-4-nitrobenzene

SECTION 16. Other information

Training advice

Provide adequate information, instruction and training for operators.

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

H302 Harmful if swallowed.
H311 Toxic in contact with skin.
H317 May cause an allergic skin reaction.
H411 Toxic to aquatic life with long lasting effects.

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.

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The information contained herein is based on the present state of our knowledge. It characterizes the product with regard to appropriate safety precautions. It does not represent a warranty of any product properties and we assume no liability for any loss or injury which may result from the use of this information. Users should conduct their own investigations to determine the suitability of the information.

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