

Chemical Safety Data Sheet MSDS / SDS

4-Chloronitrobenzene

Revision Date:2024-12-21 Revision Number:1

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

Product identifier

Product name : 4-Chloronitrobenzene
CBnumber : CB1726260
CAS : 100-00-5
EINECS Number : 202-809-6
Synonyms : 1-chloro-4-nitrobenzene,PNCB

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

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.
Uses advised against : none

Company Identification

Company : Chemicalbook
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone : 400-158-6606

SECTION 2: Hazards identification

GHS Label elements, including precautionary statements

Symbol(GHS)



Signal word

Danger

Precautionary statements

P501 Dispose of contents/container to....
P405 Store locked up.
P403+P233 Store in a well-ventilated place. Keep container tightly closed.
P391 Collect spillage. Hazardous to the aquatic environment
P311 Call a POISON CENTER or doctor/physician.
P307+P311 IF exposed: call a POISON CENTER or doctor/physician.
P301+P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.
P280 Wear protective gloves/protective clothing/eye protection/face protection.
P273 Avoid release to the environment.
P271 Use only outdoors or in a well-ventilated area.

P270 Do not eat, drink or smoke when using this product.
P264 Wash skin thoroughly after handling.
P264 Wash hands thoroughly after handling.
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P260 Do not breathe dust/fume/gas/mist/vapours/spray.
P202 Do not handle until all safety precautions have been read and understood.
P201 Obtain special instructions before use.

Hazard statements

H411 Toxic to aquatic life with long lasting effects
H373 May cause damage to organs through prolonged or repeated exposure
H372 Causes damage to organs through prolonged or repeated exposure
H370 Causes damage to organs
H361 Suspected of damaging fertility or the unborn child
H351 Suspected of causing cancer
H341 Suspected of causing genetic defects
H331 Toxic if inhaled
H320 Causes eye irritation
H311 Toxic in contact with skin
H301 Toxic if swallowed

Disposal

WARNING.Cancer - <https://oehha.ca.gov/proposition-65/chemicals/1-chloro-4-nitrobenzene>

SECTION 3: Composition/information on ingredients

Substance

Product name	: 4-Chloronitrobenzene
Synonyms	: 1-chloro-4-nitrobenzene,PNCB
CAS	: 100-00-5
EC number	: 202-809-6
MF	: C6H4ClNO2
MW	: 157.55

SECTION 4: First aid measures

Description of first aid measures

General advice

Consult a physician. Show this safety data sheet to the doctor in attendance.

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.

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

Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

Extinguishing media

Suitable extinguishing media

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

Special hazards arising from the substance or mixture

Carbon oxides, Nitrogen oxides (NO_x), Hydrogen chloride gas

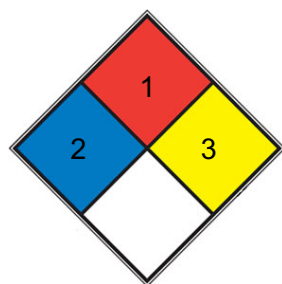
Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

Further information

No data available

NFPA 704



HEALTH 2 Intense or continued but not chronic exposure could cause temporary incapacitation or possible residual injury (e.g. [diethyl ether](#), ammonium phosphate, iodine)

FIRE 1 Materials that require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur. Includes some finely divided suspended solids that do not require heating before ignition can occur. Flash point at or above 93.3 °C (200 °F). (e.g. [mineral oil](#), ammonia)

REACT 3 Capable of detonation or explosive decomposition but requires a strong initiating source, must be heated under confinement before initiation, reacts explosively with water, or will detonate if severely shocked (e.g. [ammonium nitrate](#), cesium, hydrogen peroxide)

SPEC.

HAZ.

SECTION 6: Accidental release measures

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.

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.

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.

Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

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.

Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Store in cool place.

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

control parameter

Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

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.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0,11 mm Break through time: 480 min

Material tested: Dermatril? (KCL 740 / Aldrich Z677272, Size M)

Splash contact Material: Nitrile rubber

Minimum layer thickness: 0,11 mm Break through time: 480 min

Material tested: Dermatril? (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.

Exposure limits

Potential occupational carcinogen. NIOSH REL: IDLH 100; OSHA PEL: TWA 1.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Appearance	light yellow crystalline
Odour	No data available
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	Melting point/range: 83 - 84 °C
Initial boiling point and boiling range	242 °C at 1013 hPa
Flash point	124 °C - closed cup
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive	No data available

limits	
Vapour pressure	0.09 mm Hg (25 °C)
Vapour density	5.4 (vs air)
Relative density	1,298 g/cm ³
Water solubility	insoluble
Partition coefficient: n-octanol/water	log Pow: 2,6
Autoignition temperature	No data available
Decomposition temperature	No data available
Viscosity	No data available
Explosive properties	No data available
Oxidizing properties	No data available
Henry's Law Constant	4.90 x 10 ⁻⁶ atm·m ³ /mol at 25 °C (thermodynamic method-GC/UV spectrophotometry, Altschuh et al., 1999)

Other safety information

No data available

SECTION 10: Stability and reactivity

Reactivity

No data available

Chemical stability

Stable under recommended storage conditions.

Possibility of hazardous reactions

No data available

Conditions to avoid

No data available

Incompatible materials

Strong oxidizing agents, Strong bases

Hazardous decomposition products

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

Other decomposition products - No data available In the event of fire: see section 5

SECTION 11: Toxicological information

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.

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.

Reproductive toxicity

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.

Toxicity

LD₅₀ (skin) for rats 16 gm/kg (quoted, RTECS, 1985).

SECTION 12: Ecological information

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

Persistence and degradability

Biodegradability aerobic - Exposure time 28 d

Bioaccumulative potential

Bioaccumulation Oncorhynchus mykiss (rainbow trout) - 36 d

- 0,780 µg/l(1-Chloro-4-nitrobenzene)

Bioconcentration factor (BCF): 108

Mobility in soil

No data available

Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

Other adverse effects

Toxic to aquatic life with long lasting effects. No data available

SECTION 13: Disposal considerations

Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber. Waste material must be disposed of in accordance with the Directive on waste 2008/98/EC as well as other national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

Incompatibilities

A strong oxidizer. Reacts violently with oxidizers, combustibles, alkalis, sodium methoxide; and reducing materials.

Waste Disposal

Incineration (816°C, 0.5 second for primary combustion; 1204°C, 1.0 second for secondary combustion). The formation of elemental chlorine can be prevented through injection of steam or methane into the combustion process. nitrogen oxides may be abated through the use of thermal or catalytic devices.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

UN number

ADR/RID: 1578 IMDG: 1578 IATA: 1578

UN proper shipping name

ADR/RID: CHLORONITROBENZENES, SOLID IMDG: CHLORONITROBENZENES, SOLID

IATA: Chloronitrobenzenes, solid

14.3

Transport hazard class(es)

ADR/RID: 6.1 IMDG: 6.1

IATA: 6.1

14.4	Packaging group ADR/RID: II IMDG: II	IATA: II
14.5	Environmental hazards ADR/RID: yes IMDG Marine pollutant: yes	IATA: no
14.6	Special precautions for user No data available	

SECTION 15: Regulatory information

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

Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015:Listed. website: <https://www.mem.gov.cn/>

Measures for Environmental Management of New Chemical Substances

European Inventory of Existing Commercial Chemical Substances (EINECS):Listed. website: <https://echa.europa.eu/>

United States Toxic Substances Control Act (TSCA) Inventory:Listed. website: <https://www.epa.gov/>

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Listed. website: <https://www.mee.gov.cn/>

Vietnam National Chemical Inventory:Listed. website: <https://chemicaldata.gov.vn/>

New Zealand Inventory of Chemicals (NZIoC):Listed. website: <https://www.epa.govt.nz/>

Korea Existing Chemicals List (KECL):Listed. website: <http://ncis.nier.go.kr>

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Listed. website: <https://emb.gov.ph/>

EC Inventory:Listed.

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

References

[1] CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

[2] ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

[3] ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

[4] eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:

http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

【5】 ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>

【6】 Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

【7】 HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

【8】 IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

【9】 IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

【10】 Sigma-Aldrich, website: <https://www.sigmaaldrich.com/>

Other Information

Depending on the degree of exposure, periodic medical examination is indicated.

Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.