

Chemical Safety Data Sheet MSDS / SDS

NITROBENZENE (13C6)Revision Date:2026-03-21 Revision Number:1

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

Product name : NITROBENZENE (13C6)
CBnumber : CB5686823
CAS : 89059-37-0
Synonyms : Nitrobenzene-13C?;Nitrobenzene (13C?, 99%)

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 : 010-86108875

SECTION 2: Hazards identification**GHS Label elements, including precautionary statements**

Symbol(GHS)



Signal word Danger

Precautionary statements

P201 Obtain special instructions before use.
P273 Avoid release to the environment.
P280 Wear protective gloves/protective clothing/eye protection/face protection.

Hazard statements

H351 Suspected of causing cancer
H372 Causes damage to organs through prolonged or repeated exposure
H412 Harmful to aquatic life with long lasting effects

SECTION 3: Composition/information on ingredients**Substance**

Product name	: NITROBENZENE (13C6)
Synonyms	: Nitrobenzene-13C?;Nitrobenzene (13C?, 99%)
CAS	: 89059-37-0
MF	: C6H5NO2
MW	: 129.16

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

If inhaled

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

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Call a physician immediately.

In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed

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

The most important known symptoms and effects are described in the labelling (see section 2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

4.4 Notes to physician

No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Water Foam Carbon dioxide (CO2) 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

Carbon oxides

Nitrogen oxides (NOx)

Combustible.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

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

5.3 Advice 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.

Remove container from danger zone and cool with water. Suppress (knock down) gases/vapors/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: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition.

Evacuate the danger area, observe emergency procedures, consult an expert.

For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter 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 and 10). Take up carefully with liquid-absorbent material (e.g.

Chemizorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures

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

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

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

Storage class

Storage class (TRGS 510): 6.1A: Combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

['Component', 'CAS-No.', 'Value', 'Control parameters', 'Basis']	['Nitrobenzene- 13C6', '89059-37- 0', 'PC-TWA', '2 mg/m3', 'Occupational exposure limits for hazardous agents in the workplace - Chemical hazardous agents.']	['', 'Remarks', 'G2B - Possibly carcinogenic to humans Skin', None, None]
--	---	---

Biological occupational exposure limits

['Component', 'CAS-No.', 'Parameters', 'Value', 'Biological specimen', 'Basis']	['Nitrobenzene- 13C6', '89059-37- 0', 'Methemoglo bin', '1.5% Hb', 'In blood', 'ACGIH - Biological Exposure Indices (BEI)']	['', 'Remarks', 'During or at the end of the shift', None, None, None]
---	---	--

8.2 Exposure controls

Appropriate engineering controls

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

Personal protective equipment

Eye/face protection

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

Skin protection

required

Body Protection

protective clothing

Respiratory protection

required when vapours/aerosols are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Control of environmental exposure

Do not let product enter drains.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

a) Physical state	liquid
b) Color	Colourless
c) Odor	No data available
d) Melting point/freezing point	Melting point/range: 5 - 6 °C

e) Initial boiling point and boiling range	210 - 211 °C - lit.
f) Flammability (solid, gas)	No data available
g) Upper/lower flammability or explosive limits	Upper explosion limit: 40 %(V) Lower explosion limit: 1.8 %(V)
h) Flash point	88 °C - closed cup
i) Autoignition temperature	482 °C
j) Decomposition temperature	No data available
k) pH	8.0 - 8.5 at 1 g/l at 20 °C
l) Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
m) Water solubility	No data available
n) Partition coefficient n-octanol/water	No data available
o) Vapor pressure	0.3 hPa at 20 °C 67 hPa at 120 °C
p) Density	1.253 g/cm ³ at 25 °C
Relative density	1.253 g/mL at 25 °C
q) Relative vapor density	No data available
r) Particle characteristics	No data available
s) Explosive properties	No data available
t) Oxidizing properties	No data available
Solubility	Chloroform (Slightly), Methanol (Slightly)

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Chemical stability

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

10.2 Possibility of hazardous reactions

No data available

10.3 Conditions to avoid

Strong heating.

10.4 Incompatible materials

Strong oxidizing agents, Strong reducing agents, Strong bases

10.5 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

Acute toxicity estimate Oral - 100.1 mg/kg (Expert judgment)

LC50 Inhalation - Rat - 4 h - 2.8 mg/l - vapor

Remarks: Sense Organs and Special Senses (Nose, Eye, Ear, and Taste):Eye:Lacrimation.

Behavioral:Tremor.

Cyanosis

The value is given in analogy to the following substances: Nitrobenzene

LD50 Dermal - Rabbit - 760 mg/kg

Remarks: The value is given in analogy to the following substances: Nitrobenzene

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 24 h

Remarks: Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation

Remarks: The value is given in analogy to the following substances: Nitrobenzene

Respiratory or skin sensitization

- Mouse

Result: Did not cause sensitization on laboratory animals.

(OECD Test Guideline 429)

Remarks: The value is given in analogy to the following substances: Nitrobenzene

Germ cell mutagenicity

Test Type: unscheduled DNA synthesis assay

Test system: rat hepatocytes

Method: OECD Test Guideline 482

Result: negative

Remarks:

Test Type: Micronucleus test

Species: Mouse

Application Route: Intraperitoneal

Method: OECD Test Guideline 474

Result: negative

Remarks: The value is given in analogy to the following substances: Nitrobenzene

Carcinogenicity

Suspected human carcinogens

Reproductive toxicity

Presumed human reproductive toxicant

Specific target organ toxicity - single exposure

Classified based on available data. For more details, see section 2

Specific target organ toxicity - repeated exposure

Inhalation - Causes damage to organs through prolonged or repeated exposure.

- Blood

Remarks: The value is given in analogy to the following substances: Nitrobenzene

Aspiration hazard

Classified based on available data. For more details, see section 2

11.2 Additional Information

Repeated dose toxicity - Rat - male and female - Oral - 28 d - LOAEL (Lowest observed adverse effect level) - 5 mg/kg

Remarks: The value is given in analogy to the following substances: Nitrobenzene

Repeated dose toxicity - Rat - male and female - Inhalation - 14 d

Remarks: The value is given in analogy to the following substances: Nitrobenzene

Absorption into the body leads to the formation of methemoglobin which in sufficient concentration causes cyanosis. Onset may be delayed 2 to 4 hours or longer., Exposure to and/or consumption of alcohol may increase toxic effects., Nausea, Headache, Vomiting, To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish flow-through test LC50 - Danio rerio (zebra fish) - 92 mg/l - 96.0 h (OECD Test Guideline 203)

Remarks: The value is given in analogy to the following substances:

Nitrobenzene

Toxicity to daphnia static test EC50 - Daphnia magna (Water flea) - 35 mg/l - 48 h and other aquatic Remarks: The value is given in analogy to the following substances: invertebrates Nitrobenzene

Toxicity to algae Growth inhibition EC50 - Chlorella pyrenoidosa - 18 mg/l - 96 h (OECD Test Guideline 201)

Remarks: The value is given in analogy to the following substances:

Nitrobenzene

Toxicity to daphnia NOEC - Daphnia magna (Water flea) - 2.6 mg/l - 21 d and other aquatic Remarks: The value is given in analogy to the following substances: invertebrates(Chronic Nitrobenzene toxicity)

12.2 Persistence and degradability

No data available

12.3 Bioaccumulative potential

No data available

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 Endocrine disrupting properties

No data available

12.7 Other adverse effects

No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company.

SECTION 14: Transport information

14.1 UN number

ADR/RID: 1662

IMDG: 1662

IATA-DGR: 1662

14.2 UN proper shipping name

ADR/RID: NITROBENZENE

IMDG: NITROBENZENE

IATA-DGR: Nitrobenzene

14.3 Transport hazard class(es)

ADR/RID: 6.1

IMDG: 6.1

IATA-DGR: 6.1

14.4 Packaging group

ADR/RID: II

IMDG: II

IATA-DGR: II

14.5 Environmental hazards

ADR/RID: yes

IMDG Marine pollutant: yes

IATA-DGR: no

14.6 Special precautions for user

Based on chemical properties, choose appropriate tools and conditions of transport.

Transporting tools shall be equipped with appropriate and sufficient firefighting equipment and emergency leaking installations. If transporting by road, please go along the specified route.

14.7 Incompatible materials

Strong oxidizing agents, Strong reducing agents, Strong bases

SECTION 15: Regulatory information

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

National regulatory information

Law on the Prevention and Control of Occupational Diseases

Regulations on Safety Management of Hazardous Chemicals

Catalogue of Hazardous Chemicals : Listed

Regulations on Occupational Labor Protection in the at workplaces where Toxic

Substances Are Used

Catalogue of Highly Toxic Chemicals : Listed

Measures on the Environmental Administration of New Chemical Substances Registration

Registration/Notification number : B1A222214570

Downstream users need to comply with the conditions of safe use of the chemical, understand the environmental and health hazard and risk management measures identified on the SDS as well as the local/national regulations concerning the chemical.

Other regulations

Please pay attention on the waste treatment should also comply with local regulations requirement.

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

TWA: Time-Weighted Average

STEL: Short-Term Exposure Limit

LD50: Lethal Dose 50%

LC50: Lethal Concentration 50%

EC50: Effective Concentration 50%

PEL: Permissible Exposure Limit

TLV: Threshold Limit Value

IMDG: International Maritime Dangerous Goods Code

IATA: International Air Transport Association

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

DOT: US Department of Transportation

NFPA: National Fire Protection Association

NIOSH: National Institute for Occupational Safety and Health

OSHA: Occupational Safety and Health Administration

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.