ChemicalBook

Chemical Safety Data Sheet MSDS / SDS

NITROBENZENE-D5

Revision Date:2025-10-04 Revision Number:1

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

Product identifier

Product name	: NITROBENZENE-D5
CBnumber	: CB7360620
CAS	: 4165-60-0
EINECS Number	: 224-014-3
Synonyms	: nitrobenzene-d5,1,2,3,4,5-pentadeuterio-6-nitrobenzene

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

P405 Store locked up.

P403+P233 Store in a well-ventilated place. Keep container tightly closed.

P337+P313 IF eye irritation persists: Get medical advice/attention.

P330 Rinse mouth.

P320 Specific treatment is urgent (see … on this label).

P308+P313 IF exposed or concerned: Get medical advice/attention.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continuerinsing.

P304+P340 IF INHALED: Remove victim to fresh air and Keep at rest in a position comfortable for breathing.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P201 Obtain special instructions before use.

Hazard statements

H412 Harmful to aquatic life with long lasting effects

H411 Toxic to aquatic life with long lasting effects

H401 Toxic to aquatic life

H373 May cause damage to organs through prolonged or repeated exposure

H372 Causes damage to organs through prolonged or repeated exposure

H361 Suspected of damaging fertility or the unborn child

H351 Suspected of causing cancer

H336 May cause drowsiness or dizziness

H335 May cause respiratory irritation

H330 Fatal if inhaled

H319 Causes serious eye irritation

H315 Causes skin irritation

H310 Fatal in contact with skin

H300 Fatal if swallowed

H227 Combustible liquid

SECTION 3: Composition/information on ingredients

Substance

Product name	: NITROBENZENE-D5
Synonyms	: nitrobenzene-d5,1,2,3,4,5-pentadeuterio-6-nitrobenzene
CAS	: 4165-60-0
EC number	: 224-014-3
MF	: C6D5NO2
MW	: 128.14

SECTION 4: First aid measures

Description of first aid measures

General advice

Consult a physician. Show this material 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

Do NOT induce vomiting. 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.

Unsuitable extinguishing media

Do NOT use water jet.

Special hazards arising from the substance or mixture

Carbon oxides Nitrogen oxides (NOx)

Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

Further information

Use water spray to cool unopened containers.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Wear respiratory protection. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of
vapors accumulating to form explosive concentrations. Vapors can accumulate in low areas.
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

Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13). 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

Advice on safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapor or mist.

Advice on protection against fire and explosion

Keep away from sources of ignition - No smoking.Take measures to prevent the build up of electrostatic charge.

Hygiene measures

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

For precautions see section 2.2.

Conditions for safe storage, including any incompatibilities

Storage conditions

Keep container tightly closed in a dry and well-ventilated place. Containers which are

opened must be carefully resealed and kept upright to prevent leakage. Store in cool place.

Specific end use(s)

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

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SECTION 8: Exposure controls/personal protection

control parameter

Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

Exposure controls

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.

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 respirator with multi-purpose combination (US) or type

ABEK (EN 14387) 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.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Appearance	liquid
Odour	No data available
Odour Threshold	No data available
pH	8.1 (1g/l, H2O, 20℃)
Melting point/freezing point	6°C
Initial boiling point and boiling range	88 °C at 16 hPa - lit.
Flash point	88 °C
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	Upper explosion limit: 40 %(V) Lower explosion limit: 1,8 %(V)
Vapour pressure	No data available
Vapour density	No data available
Relative density	1,253 g/cm3 at 25 °C - lit. No data available
Water solubility	1.9g/l
Partition coefficient: n-octanol/water	No data available
Autoignition temperature	No data available
Decomposition temperature	No data available
Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
Explosive properties	No data available
Oxidizing properties	No data available

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

Heat, flames and sparks.

Incompatible materials

No data available

Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

Information on toxicological effects

Acute toxicity

Oral

Acute toxicity estimate Oral - 100,1 mg/kg (Expert judgment)

LC50 Inhalation - Rat - 4 h - 2,8 mg/l Remarks: (RTECS)

Inhalation: absorption Dermal: absorption

LD50 Dermal - Rabbit - 760 mg/kg Remarks: (ECHA)

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

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation Remarks: (ECHA)

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

Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation Remarks: (ECHA)

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

Respiratory or skin sensitization

Remarks: (IUCLID)

The value is given in analogy to the following substances: Nitrobenzene Local lymph node assay (LLNA) - Mouse

Result: Does not cause skin sensitization. (OECD Test Guideline 429)

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

Germ cell mutagenicity

Test Type: Micronucleus test Species: Mouse

Cell type: Bone marrow

Application Route: Intraperitoneal injection Method: OECD Test Guideline 474

Result: negative

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

Test Type: unscheduled DNA synthesis assay Species: Rat

Cell type: Liver cells Application Route: Oral

Method: OECD Test Guideline 486 Result: negative

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

Carcinogenicity

No data available

Reproductive toxicity

May damage fertility.

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

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

Aspiration hazard

No data available

SECTION 12: Ecological information

Toxicity

Toxicity to fish

flow-through test LC50 - Danio rerio (zebra fish) - 92,2 mg/l - 96 h (OECD Test Guideline 203)

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

Toxicity to daphnia and other aquatic invertebrates

static test EC50 - Daphnia magna (Water flea) - 35 mg/l - 48 h (OECD Test Guideline 202)

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

Toxicity to algae

IC5 - Scenedesmus quadricauda (Green algae) - 33 mg/l Remarks: (Lit.)

IC50 - Chlorella pyrenoidosa - 18 mg/l - 96 h Remarks: (IUCLID)

static test ErC50 - 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 bacteria

static test EC20 - activated sludge - 1.000 mg/l - 30 min

(OECD Test Guideline 209)

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

Persistence and degradability

Biodegradability Result: 3,3 % - Not readily biodegradable.

(OECD Test Guideline 301C)

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

Bioaccumulative potential

No data available

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. Discharge into the environment must be avoided.

SECTION 13: Disposal considerations

Waste treatment methods

Product

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

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

UN number

ADR/RID: 1662 IMDG: 1662

UN proper shipping name

ADR/RID: NITROBENZENE IMDG: NITROBENZENE IATA: Nitrobenzene

Transport hazard class(es)

ADR/RID: 6.1 IMDG: 6.1 IATA: 6.1

Packaging group

ADR/RID: II IMDG: II IATA: II

Environmental hazards

ADR/RID: yes IMDG Marine pollutant: yes IATA: no

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:Not Listed. website: https://www.mem.gov.cn/

Measures for Environmental Management of New Chemical Substances

Vietnam National Chemical Inventory:Not Listed. website: https://chemicaldata.gov.vn/

United States Toxic Substances Control Act (TSCA) Inventory:Not Listed. website: https://www.epa.gov/

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Not Listed. website: https://emb.gov.ph/

Korea Existing Chemicals List (KECL):Not Listed. website: http://ncis.nier.go.kr

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Not Listed. website: https://www.mee.gov.cn/

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

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

EC Inventory:Listed.

SECTION 16: Other information

Abbreviations and acronyms

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

CAS: Chemical Abstracts Service

EC50: Effective Concentration 50%

IATA: International Air Transportation Association

IMDG: International Maritime Dangerous Goods

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

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

STEL: Short term exposure limit

TWA: Time Weighted Average

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/