

SAFETY DATA SHEET

Version 6.8
Revision Date 10/08/2021
Print Date 12/06/2021**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**Product name : Nitrobenzene-d₅Product Number : 151955
Brand : Aldrich
CAS-No. : 4165-60-0**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 sheetCompany : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATESTelephone : +1 314 771-5765
Fax : +1 800 325-5052**1.4 Emergency telephone**Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-
527-3887 CHEMTREC (International) 24
Hours/day; 7 Days/week**SECTION 2: Hazards identification****2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**Flammable liquids (Category 4), H227
Acute toxicity, Oral (Category 3), H301
Acute toxicity, Inhalation (Category 3), H331
Acute toxicity, Dermal (Category 3), H311
Carcinogenicity (Category 2), H351
Reproductive toxicity (Category 2), H361
Specific target organ toxicity - repeated exposure (Category 1), H372
Short-term (acute) aquatic hazard (Category 2), H401
Long-term (chronic) aquatic hazard (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)

H227

Combustible liquid.

H301 + H311 + H331

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

H351

Suspected of causing cancer.

H361

Suspected of damaging fertility or the unborn child.

H372

Causes damage to organs through prolonged or repeated exposure.

H411

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.

P210

Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.

P260

Do not breathe dust/ fume/ gas/ mist/ vapors/ 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/ eye protection/ face protection.

P301 + P310 + P330

IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth.

P302 + P352 + P312

IF ON SKIN: Wash with plenty of water. Call a POISON CENTER/ doctor if you feel unwell.

P304 + P340 + P311

IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor.

P308 + P313

IF exposed or concerned: Get medical advice/ attention.

P362

Take off contaminated clothing and wash before reuse.

P370 + P378

In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.

P391

Collect spillage.

P403 + P233

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

P403 + P235

Store in a well-ventilated place. Keep cool.

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

SECTION 3: Composition/information on ingredients

3.1 Substances

Synonyms : Pentadeuteronitrobenzene

Formula : C₆D₅NO₂

Molecular weight : 128.15 g/mol

CAS-No. : 4165-60-0

Aldrich - 151955

Page 2 of 12

EC-No. : 224-014-3

Component	Classification	Concentration
nitrobenzene-ds	Flam. Liq. 4; Acute Tox. 3; Carc. 2; Repr. 1B; STOT RE 1; Aquatic Acute 3; Aquatic Chronic 3; H227, H301, H331, H311, H351, H360, H372, H402, H412	<= 100 %

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

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

Consult a physician. Show this material 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

Do NOT induce vomiting. 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

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

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

Unsuitable extinguishing media

Do NOT use water jet.

5.2 Special hazards arising from the substance or mixture

Carbon oxides
Nitrogen oxides (NO_x)

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

Use water spray to cool unopened containers.

SECTION 6: Accidental release measures

6.1 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.

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

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.

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

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.

7.2 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.

Storage class

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

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
nitrobenzene-d ₅	4165-60-0	TWA	1 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Confirmed animal carcinogen with unknown relevance to humans Danger of cutaneous absorption		
		TWA	1 ppm 5 mg/m ³	USA. NIOSH Recommended Exposure Limits
		Potential for dermal absorption		
		TWA	1 ppm 5 mg/m ³	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		Skin designation		
		TWA	1 ppm 5 mg/m ³	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		Skin notation		
		PEL	1 ppm 5 mg/m ³	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		

Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
nitrobenzene-d ₅	4165-60-0	Methemoglobin	1.5% Hb	In blood	ACGIH - Biological Exposure Indices (BEI)
	Remarks	During or at the end of the shift			

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.

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

9.1 Information on basic physical and chemical properties

- | | |
|---|---|
| a) Appearance | Form: liquid |
| b) Odor | No data available |
| c) Odor Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | No data available |
| f) Initial boiling point and boiling range | 88 °C 190 °F at 16 hPa - lit. |
| g) Flash point | 88 °C (190 °F) |
| h) Evaporation rate | No data available |
| i) Flammability (solid, gas) | No data available |
| j) Upper/lower flammability or explosive limits | Upper explosion limit: 40 %(V)
Lower explosion limit: 1.8 %(V) |
| k) Vapor pressure | No data available |
| l) Vapor density | No data available |
| m) Density | 1.253 g/cm ³ at 25 °C (77 °F) - lit. |
| Relative density | No data available |
| n) Water solubility | No data available |
| o) Partition coefficient: n-octanol/water | No data available |

- | | |
|------------------------------|-------------------|
| p) Autoignition 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

SECTION 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

Heat, flames and sparks.

10.5 Incompatible materials

No data available

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

Oral: absorption

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

Sensitisation test: - Guinea pig

Result: negative

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

Suspected of causing cancer.

IARC: 2B - Group 2B: Possibly carcinogenic to humans (nitrobenzene-d₅)

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.

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

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

11.2 Additional Information

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

Aldrich - 151955

Page 8 of 12

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.

After absorption:

agitation
CNS disorders
Drowsiness
Unconsciousness
collapse
Coma

Symptoms may be delayed.

Effect potentiated by: ethanol

Other information

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

Further data:

Other dangerous properties can not be excluded.

This substance should be handled with particular care.

Spleen. -

SECTION 12: Ecological information

12.1 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)

Aldrich - 151955

Page 9 of 12

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

12.2 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

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

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

Toxic to aquatic life with long lasting effects.

Discharge into the environment must be avoided.

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. This combustible material may be burned in a chemical incinerator equipped with an afterburner and scrubber. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information**DOT (US)**

UN number: 1662 Class: 6.1 Packing group: II
Proper shipping name: Nitrobenzene
Reportable Quantity (RQ): 1000 lbs
Reportable Quantity (RQ): 1000 lbs
1) Marine pollutant: yes Poison Inhalation Hazard: No

IMDG

UN number: 1662 Class: 6.1 Packing group: II EMS-No: F-A, S-A
Proper shipping name: NITROBENZENE
Marine pollutant : yes

IATA

UN number: 1662 Class: 6.1 Packing group: II
Proper shipping name: Nitrobenzene

SECTION 15: Regulatory information**SARA 302 Components**

The following components are subject to reporting levels established by SARA Title III, Section 302:

	CAS-No.	Revision Date
nitrobenzene-d5	4165-60-0	2008-11-03

SARA 313 Components

The following components are subject to reporting levels established by SARA Title III, Section 313:

	CAS-No.	Revision Date
nitrobenzene-d5	4165-60-0	2008-11-03

SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard, Chronic Health Hazard

Reportable Quantity : D036 lbs

Massachusetts Right To Know Components

No components are subject to the Massachusetts Right to Know Act.

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
nitrobenzene-d5	4165-60-0	2008-11-03

	CAS-No.	Revision Date
nitrobenzene-d5	4165-60-0	2008-11-03

New Jersey Right To Know Components

	CAS-No.	Revision Date
nitrobenzene-d5	4165-60-0	2008-11-03

California Prop. 65 Components

This product does not contain any chemicals known to the State of California to cause cancer, birth, or any other reproductive defects.

SECTION 16: Other information

Further information

Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact mlsbranding@sial.com.

Version: 6.8

Revision Date: 10/08/2021

Print Date: 12/06/2021