

SAFETY DATA SHEET

Version 3.11
Revision Date 09/23/2016
Print Date 10/10/2017

1. PRODUCT AND COMPANY IDENTIFICATION**1.1 Product identifiers**

Product name : Nitrobenzene-d₅

Product Number : 442718

Brand : Supelco

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 sheet

Company : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA

Telephone : +1 800-325-5832

Fax : +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

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

Acute aquatic toxicity (Category 2), H401

Chronic aquatic toxicity (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/ vapours/ 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 soap and water. Call a POISON CENTER or doctor/ physician 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

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms	: Pentadeuteronitrobenzene
Formula	: C ₆ D ₅ NO ₂
Molecular weight	: 128.14 g/mol
CAS-No.	: 4165-60-0
EC-No.	: 224-014-3

Hazardous components

Component	Classification	Concentration
Nitrobenzene-d5 Included in the Candidate List of Substances of Very High Concern (SVHC) according to Regulation (EC) No. 1907/2006 (REACH)		
	Flam. Liq. 4; Acute Tox. 3; Carc. 2; Repr. 2; STOT RE 1; Aquatic Acute 2; Aquatic Chronic 2; H227, H301 + H311 + H331, H351, H361, H372, H411	<= 100 %

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

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice

Consult a physician. Show this 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

5. FIREFIGHTING MEASURES**5.1 Extinguishing media****Suitable extinguishing media**

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

5.2 Special hazards arising from the substance or mixture

No data available

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.

6. ACCIDENTAL RELEASE MEASURES**6.1 Personal precautions, protective equipment and emergency procedures**

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

Vapours 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 an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13). Keep in suitable, closed containers for disposal.

6.4 Reference to other sections

For disposal see section 13.

7. HANDLING AND STORAGE**7.1 Precautions for safe handling**

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

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

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

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.

7.3 Specific end use(s)

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

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
Nitrobenzene-d5	4165-60-0	TWA	1.000000 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Methemoglobinemia Substances for which there is a Biological Exposure Index or Indices (see BEI® section) Confirmed animal carcinogen with unknown relevance to humans Danger of cutaneous absorption		
		TWA	1 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Methemoglobinemia Confirmed animal carcinogen with unknown relevance to humans Danger of cutaneous absorption		
		TWA	1.000000 ppm 5.000000 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		Skin designation The value in mg/m3 is approximate.		
		TWA	1.000000 ppm 5.000000 mg/m3	USA. NIOSH Recommended Exposure Limits
		Potential for dermal absorption		
		PEL	1 ppm 5 mg/m3	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-d5	4165-60-0	Total p-nitrophenol	5mg/g Creatinine	Urine	ACGIH - Biological Exposure Indices (BEI)
	Remarks	End of shift at end of workweek			
		Methemoglobin	1.5% Hb	In blood	ACGIH - Biological Exposure Indices (BEI)
		End of shift (As soon as possible after exposure ceases)			
		Methemoglobin	1.5% Hb	In blood	ACGIH - Biological Exposure Indices (BEI)
		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.

9. PHYSICAL AND CHEMICAL PROPERTIES**9.1 Information on basic physical and chemical properties**

a) Appearance	Form: liquid, clear Colour: light yellow
b) Odour	No data available
c) Odour 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 (12 mmHg) - lit.
g) Flash point	88.0 °C (190.4 °F) - closed cup
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	No data available
k) Vapour pressure	No data available
l) Vapour density	No data available
m) Relative density	1.253 g/cm ³ at 25 °C (77 °F)
n) Water solubility	No data available
o) Partition coefficient: n-octanol/water	No data available
p) Auto-ignition 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

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

Strong oxidizing agents, Strong reducing agents, Strong bases

10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NOx)

Other decomposition products - No data available

In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

No data available

Inhalation: No data available

Dermal: No data available

No data available

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitisation

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

This product is or contains a component that has been reported to be possibly carcinogenic based on its IARC, ACGIH, NTP, or EPA classification.

Limited evidence of carcinogenicity in animal studies

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

NTP: Reasonably anticipated to be a human carcinogen (Nitrobenzene-d5)

OSHA: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

Reproductive toxicity

Suspected human reproductive toxicant

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

Causes damage to organs through prolonged or repeated exposure.

Aspiration hazard

No data available

Additional Information

RTECS: Not available

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.

Spleen. -

12. ECOLOGICAL INFORMATION**12.1 Toxicity**

No data available

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 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.

13. DISPOSAL CONSIDERATIONS**13.1 Waste treatment methods****Product**

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

Contaminated packaging

Dispose of as unused product.

14. TRANSPORT INFORMATION**DOT (US)**

UN number: 1662 Class: 6.1 Packing group: II

Proper shipping name: Nitrobenzene

Reportable Quantity (RQ): 1000 lbs

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

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	2007-07-01

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	2007-07-01

SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

	CAS-No.	Revision Date
Nitrobenzene-d5	4165-60-0	2007-07-01

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Nitrobenzene-d5	4165-60-0	2007-07-01

New Jersey Right To Know Components

	CAS-No.	Revision Date
Nitrobenzene-d5	4165-60-0	2007-07-01

California Prop. 65 Components

WARNING! This product contains a chemical known to the State of California to cause cancer.

	CAS-No.	Revision Date
Nitrobenzene-d5	4165-60-0	2010-06-11

WARNING: This product contains a chemical known to the State of California to cause birth defects or other reproductive harm.

	CAS-No.	Revision Date
Nitrobenzene-d5	4165-60-0	2010-06-11

16. OTHER INFORMATION

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

Acute Tox.	Acute toxicity
Aquatic Acute	Acute aquatic toxicity
Aquatic Chronic	Chronic aquatic toxicity
Carc.	Carcinogenicity
Flam. Liq.	Flammable liquids
H227	Combustible liquid.
H301	Toxic if swallowed.
H301 + H311 + H331	Toxic if swallowed, in contact with skin or if inhaled
H311	Toxic in contact with skin.
H331	Toxic if inhaled.
H351	Suspected of causing cancer.

HMIS Rating

Health hazard:	2
Chronic Health Hazard:	*
Flammability:	2
Physical Hazard	0

NFPA Rating

Health hazard:	2
Fire Hazard:	2
Reactivity Hazard:	0

Further information

Copyright 2016 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.

Preparation Information

Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

Version: 3.11

Revision Date: 09/23/2016

Print Date: 10/10/2017