

SAFETY DATA SHEET

Version 6.0
Revision Date 07/13/2018
Print Date 10/17/2019

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

Product name : Nitrobenzene-c1ccccc1[N+](=O)[O-]

Product Number : 490369

Brand : Aldrich

CAS-No. : 89059-37-0

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 Inc.
3050 Spruce Street
ST. LOUIS MO 63103
UNITED STATES

Telephone : +1 314 771-5765

Fax : +1 800 325-5052

1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887

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

Rapidly absorbed through skin.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Formula : $^{13}\text{C}_6\text{H}_5\text{NO}_2$

Molecular weight : 129.01 g/mol

CAS-No. : 89059-37-0

Hazardous components

Component	Classification	Concentration
Nitrobenzene-13C6		
	Flam. Liq. 4; Acute Tox. 3; Carc. 2; Repr. 1B; STOT RE 1; Aquatic Acute 3; Aquatic Chronic 3; H227, H301 + H311 + H331, H351, H360,	<= 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

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

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

Carbon oxides, Nitrogen oxides (NOx)

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.

Store under inert gas. hygroscopic

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

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
Nitrobenzene-13C6	89059-37-0	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	1.000000 ppm 5.000000 mg/m3	USA. NIOSH Recommended Exposure Limits
		Potential for dermal 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 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Methemoglobinemia Confirmed animal carcinogen with unknown relevance to humans Danger of cutaneous absorption		
		PEL	1 ppm 5 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		
		TWA	1 ppm 5 mg/m3	USA. NIOSH Recommended Exposure Limits
		Potential for dermal absorption		
		TWA	1 ppm 5 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		Skin designation The value in mg/m3 is approximate.		

Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
Nitrobenzene-13C6	89059-37-0	Total p-nitrophenol	5.0000 mg/g	In urine	ACGIH - Biological Exposure Indices (BEI)
	Remarks	End of shift at end of workweek			
		Methemoglobin in	1.500 %	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.

Full contact

Material: butyl-rubber

Minimum layer thickness: 0.3 mm

Break through time: 480 min

Material tested: Butoject® (KCL 897 / Aldrich Z677647, Size M)

Splash contact

Material: Nature latex/chloroprene

Minimum layer thickness: 0.6 mm

Break through time: 30 min

Material tested: Lapren® (KCL 706 / Aldrich Z677558, 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 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 |
| b) Odour | No data available |
| c) Odour Threshold | No data available |
| d) pH | 8.0 - 8.5 at 1 g/l at 20 °C (68 °F) |
| e) Melting point/freezing point | Melting point/range: 5 - 6 °C (41 - 43 °F) |
| f) Initial boiling point and boiling range | 210 - 211 °C (410 - 412 °F) - lit. |

g) Flash point	88 °C (190 °F) - closed cup
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) Vapour pressure	0.3 hPa at 20 °C (68 °F) 67 hPa at 120 °C(248 °F)
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	482 °C (900 °F)
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 (NO_x)

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

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

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:

LD50 Dermal - Rabbit - 760 mg/kg

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

No data available

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 24 h

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

Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation

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

Respiratory or skin sensitisation

- Mouse

Result: Did not cause sensitisation on laboratory animals.

(OECD Test Guideline 429)

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

Germ cell mutagenicity

unscheduled DNA synthesis assay

rat hepatocytes

Result: negative

The value is given in analogy to the following substances:

OECD Test Guideline 474

Mouse - male and female

Result: negative

The value is given in analogy to the following substances:

Carcinogenicity

Suspected human carcinogens

IARC: 2B - Group 2B: Possibly carcinogenic to humans (Nitrobenzene-13C6)

NTP: RAHC - Reasonably anticipated to be a human carcinogen (Nitrobenzene-13C6)

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

Presumed human reproductive toxicant

Specific target organ toxicity - single exposure**Specific target organ toxicity - repeated exposure**

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

The value is given in analogy to the following substances:

Inhalation - Blood

Aspiration hazard**Additional Information**

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

The value is given in analogy to the following substances:

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

The value is given in analogy to the following substances:

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.

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to fish	flow-through test LC50 - Danio rerio (zebra fish) - 92 mg/l - 96.0 h(Nitrobenzene-13C6) (OECD Test Guideline 203) Remarks: The value is given in analogy to the following substances:
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 35 mg/l - 48 h(Nitrobenzene-13C6) Remarks: The value is given in analogy to the following substances:
Toxicity to algae	Growth inhibition EC50 - Chlorella pyrenoidosa - 18 mg/l - 96 h(Nitrobenzene-13C6) (OECD Test Guideline 201) Remarks: The value is given in analogy to the following substances:

12.2 Persistence and degradability

12.3 Bioaccumulative potential

12.4 Mobility in soil

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: no

Poison Inhalation Hazard: No

ALL INNER PACKAGINGS MUST BE IN METAL CANS FOR FXG

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
ALL INNER PACKAGINGS MUST BE IN METAL CANS FOR FX AIR

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-13C6	89059-37-0	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-13C6	89059-37-0	2008-11-03

SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

	CAS-No.	Revision Date
Nitrobenzene-13C6	89059-37-0	2008-11-03

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Nitrobenzene-13C6	89059-37-0	2008-11-03

New Jersey Right To Know Components

	CAS-No.	Revision Date
Nitrobenzene-13C6	89059-37-0	2008-11-03

California Prop. 65 Components

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

	CAS-No.	Revision Date
Nitrobenzene-13C6	89059-37-0	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-13C6	89059-37-0	2010-06-11

16. OTHER INFORMATION

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

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.
H360	May damage fertility or the unborn child.
H361	Suspected of damaging fertility or the unborn child.
H372	Causes damage to organs through prolonged or repeated exposure.
H372	Causes damage to organs (/*_ORG_REP_INHA*/) through prolonged or repeated exposure if inhaled.
H401	Toxic to aquatic life.
H411	Toxic to aquatic life with long lasting effects.
H412	Harmful to aquatic life with long lasting effects.

Further information

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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

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