SAFETY DATA SHEET

Version 6.13
Revision Date 09/08/2024
Print Date 09/09/2024

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

1.1 Product identifiers

Product name : Nitrobenzene

Product Number : 252379
Brand : SIGALD
Index-No. : 609-003-00-7
CAS-No. : 98-95-3

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone : +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 1B), H360
Specific target organ toxicity - repeated exposure, Inhalation (Category 1), Blood, H372
Short-term (acute) aquatic hazard (Category 3), H402
Long-term (chronic) aquatic hazard (Category 3), H412

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 Statements

H227	Combustible liquid.
H301 + H311 + H331	Toxic if swallowed, in contact with skin or if inhaled.
H351	Suspected of causing cancer.
H360	May damage fertility or the unborn child.
H372	Causes damage to organs (Blood) through prolonged or repeated exposure if inhaled.
H412	Harmful to aquatic life with long lasting effects.

Precautionary Statements

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 mist or vapors.
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.
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.

SECTION 3: Composition/information on ingredients

3.1 Substances

Formula	:	$C_6H_5NO_2$
Molecular weight	:	123.11 g/mol
CAS-No.	:	98-95-3
EC-No.	:	202-716-0
Index-No.	:	609-003-00-7

Component	Classification	Concentration
Nitrobenzene		
	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
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 2.2) 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
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.

5.4 Further information
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.

Store under nitrogen.

Storage class
Storage class (TRGS 510): 6.1A: 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	98-95-3	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/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		

		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	98-95-3	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
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
This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).
Full contact
Material: butyl-rubber
Minimum layer thickness: 0.7 mm
Break through time: 480 min
Material tested:Butoject® (KCL 898)

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).
Splash contact
Material: Latex gloves
Minimum layer thickness: 0.6 mm
Break through time: 30 min
Material tested:Lapren® (KCL 706 / Aldrich Z677558, Size M)

Body Protection
protective clothing

Respiratory protection
Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds

The entrepeneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.
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

9.1 Information on basic physical and chemical properties

a)	Appearance	Form: liquid, oily Color: colorless, yellow
b)	Odor	pungent
c)	Odor Threshold	0.004 ppm
d)	pH	8.0 - 8.5 at 1.00000 g/l at 20.0 °C (68.0 °F)
e)	Melting point/freezing point	Melting point/ range: 5 - 6 °C (41 - 43 °F) - lit.
f)	Initial boiling point and boiling range	210 - 211 °C 410 - 412 °F - lit.
g)	Flash point	88 °C (190 °F) - closed cup - c.c.
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	0.2 hPa at 20 °C (68 °F)
l)	Vapor density	4.1
m)	Density	1.196 g/cm3 at 25 °C (77 °F) - lit.
	Relative density	1.220 °C
n)	Water solubility	1.9 g/l at 20 °C (68 °F) - Regulation (EC) No. 440/2008, Annex, A.6
o)	Partition coefficient: n-octanol/water	log Pow: 1.86 at 24.5 °C (76.1 °F) - Bioaccumulation is not expected.
p)	Autoignition temperature	480 °C (896 °F) at 1,013 hPa - DIN 51794
q)	Decomposition temperature	> 380 °C (> 716 °F) -

r)	Viscosity	No data available
s)	Explosive properties	Not classified as explosive.
t)	Oxidizing properties	none

9.2 Other safety information

Surface tension	43.4 mN/m at 20.0 °C (68.0 °F)
Relative vapor density	4.1

SECTION 10: Stability and reactivity

10.1 Reactivity

Forms explosive mixtures with air on intense heating.
A range from approx. 15 Kelvin below the flash point is to be rated as critical.

10.2 Chemical stability

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

10.3 Possibility of hazardous reactions

Risk of explosion with:
Alkali metals
bases
aluminium chloride
ammonium nitrate
anilines
chlorosulfonic acid
glycerol
Potassium
sodium
Sodium hydroxide
Potassium hydroxide
nitrating acid
fuming sulfuric acid
Strong oxidizing agents
perchlorates
Peroxides
Reducing agents
Nitric acid
conc. sulfuric acid
nitrogen oxides
sodium chlorate
peroxodisulfuric acid
phosphorus pentachloride
silver perchlorate
tetranitromethane
uranium perchlorate
phenol
with
aluminium chloride

Generates dangerous gases or fumes in contact with:
hydrides
metallic chlorides
Heat.
Violent reactions possible with:
organometallic compounds

10.4 Conditions to avoid
Strong heating.

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
Acute toxicity estimate Oral - 100 mg/kg
(Expert judgment)
Remarks: Blood:Methemoglobinemia-Carboxyhemoglobin.
(Regulation (EC) No 1272/2008, Annex VI)
LC50 Inhalation - Rat - 4 h - 2.81 mg/l - vapor

Remarks: Sense Organs and Special Senses (Nose, Eye, Ear, and Taste):Eye:Lacrimation.
Behavioral:Tremor.
(RTECS)
LD50 Dermal - Rabbit - 760 mg/kg
Remarks: (ECHA)

Skin corrosion/irritation
Skin - Rabbit
Result: No skin irritation - 24 h
Remarks: (ECHA)

Serious eye damage/eye irritation
Eyes - Rabbit
Result: No eye irritation
Remarks: (ECHA)

Respiratory or skin sensitization
Local lymph node assay (LLNA) - Mouse
Result: negative
(OECD Test Guideline 429)

Germ cell mutagenicity
Test Type: Ames test
Test system: Salmonella typhimurium
Metabolic activation: with and without metabolic activation
Result: negative

Remarks: (ECHA)

Test Type: Micronucleus test
Species: Mouse
Cell type: Bone marrow
Application Route: Intraperitoneal injection
Method: OECD Test Guideline 474
Result: negative

Test Type: unscheduled DNA synthesis assay
Species: Rat
Cell type: Liver cells
Application Route: Oral
Method: OECD Test Guideline 486
Result: negative

Carcinogenicity
Suspected of causing cancer.

IARC:	2B - Group 2B: Possibly carcinogenic to humans (Nitrobenzene)
NTP:	RAHC - Reasonably anticipated to be a human carcinogen (Nitrobenzene)
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
Inhalation - Causes damage to organs through prolonged or repeated exposure.
- Blood
Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Aspiration hazard
No data available

11.2 Additional Information

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

RTECS: DA6475000
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.
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

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish	flow-through test LC50 - Danio rerio (zebra fish) - 92 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 35 mg/l - 48 h Remarks: (ECHA)
Toxicity to algae	static test ErC50 - Chlorella pyrenoidosa - 18 mg/l - 96 h (OECD Test Guideline 201)
Toxicity to bacteria	static test EC20 - activated sludge - 1,000 mg/l - 30 min (OECD Test Guideline 209)
Toxicity to fish(Chronic toxicity)	flow-through test LC50 - Oncorhynchus mykiss (rainbow trout) - 0.002 mg/l - 23 d Remarks: (ECHA)
Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity)	semi-static test NOEC - Daphnia magna (Water flea) - 2.6 mg/l - 21 d

12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 28 d Result: 50 % - Readily biodegradable. (OECD Test Guideline 301F)

12.3 Bioaccumulative potential

Bioaccumulation	Cyprinus carpio (Carp) - 42 d at 25 °C - 0.125 mg/l(Nitrobenzene) Bioconcentration factor (BCF): 3.1 - 4.8 (OECD Test Guideline 305C)

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
Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

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
Reportable Quantity (RQ): 100 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

SECTION 15: Regulatory information

CERCLA Reportable Quantity

Components	CAS-No.	Component RQ (lbs)	Calculated product RQ (lbs)
Nitrobenzene	98-95-3	1000	1000
Nitrobenzene	98-95-3	1000	1000 (D036)
Nitrobenzene	98-95-3	100	100 (F004)

SARA 304 Extremely Hazardous Substances Reportable Quantity

Components	CAS-No.	Component RQ (lbs)	Calculated product RQ (lbs)
Nitrobenzene	98-95-3	1000	1000

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

Components	CAS-No.	Component TPQ (lbs)
Nitrobenzene	98-95-3	10000

SARA 311/312 : Fire Hazard

Hazards		Acute Health Hazard Chronic Health Hazard
SARA 313	:	The following components are subject to reporting levels established by SARA Title III, Section 313:

Nitrobenzene	98-95-3	>= 90 - <= 100 %

US State Regulations

Massachusetts Right To Know

Nitrobenzene	98-95-3

Pennsylvania Right To Know

Nitrobenzene	98-95-3

Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Product does not contain any listed chemicals

Washington Chemicals of High Concern

Product does not contain any listed chemicals

California Prop. 65

WARNING: This product can expose you to chemicals including Nitrobenzene, which is/are known to the State of California to cause cancer and birth defects or other reproductive harm. For more information go to www.P65Warnings.ca.gov.

The ingredients of this product are reported in the following inventories:

TSCA : All substances listed as active on the TSCA inventory

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16: Other information

Further information

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. 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.