

Safety Data Sheet

Nitrobenzene-d5

Classification acc. to 29 CFR 1910.1200

Version number: GHS 3.0
Replaces version of: 02.02.2023 (GHS 2)

Revision: 10.06.2025

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

1.1 Product identifier

Identification of the substance	Nitrobenzene-d5
CAS number	4165-60-0
Alternative name(s)	1-nitro(² H ₅)benzene

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

Relevant identified uses	laboratory and analytical use laboratory chemical
HS code	2845.90.

1.3 Details of the supplier of the safety data sheet

Zeochem AG Joweid 5, CH-8630 Rüti Switzerland	Telephone: +41 44 922 93 93 e-Mail: info@zeochem.com Website: https://www.zeochem.com
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1.4 Emergency telephone number

Poison centre		
Country	Name	Telephone
Switzerland	Toxzentrum Zürich / Tox. Info Suisse	+41 44 251 51 51 / CH: 145 - 24h/7d
United States	CHEMTREC USA	+1 800 424 9300 - 24h/7d

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification acc. to GHS

Section	Hazard class	Category	Hazard class and category	Hazard statement
2.6	flammable liquid	4	Flam. Liq. 4	H227
3.1O	acute toxicity (oral)	4	Acute Tox. 4	H302
3.1D	acute toxicity (dermal)	3	Acute Tox. 3	H311
3.1I	acute toxicity (inhal.)	3	Acute Tox. 3	H331
3.6	carcinogenicity	2	Carc. 2	H351
3.7	reproductive toxicity	1B	Repr. 1B	H360F
3.9	specific target organ toxicity - repeated exposure	1	STOT RE 1	H372
4.1A	hazardous to the aquatic environment - acute hazard	3	Aquatic Acute 3	H402
4.1C	hazardous to the aquatic environment - chronic hazard	3	Aquatic Chronic 3	H412

For full text of abbreviations: see SECTION 16.

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The most important adverse physicochemical, human health and environmental effects



Delayed or immediate effects can be expected after short or long-term exposure. The product is combustible and can be ignited by potential ignition sources. Spillage and fire water can cause pollution of watercourses.

2.2 Label elements

Labelling

- Signal word danger

2.2.1.2 Pictograms

GHS06, GHS08	 
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Hazard statements	
H227	combustible liquid
H302	harmful if swallowed
H311+H331	toxic in contact with skin or if inhaled
H351	suspected of causing cancer
H360F	may damage fertility
H372	causes damage to organs through prolonged or repeated exposure
H412	harmful to aquatic life with long lasting effects

Precautionary statements	
P201	obtain special instructions before use
P210	keep away from heat/sparks/open flames/hot surfaces. No smoking
P260	do not breathe dust/fume/gas/mist/vapours/spray
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
P302+P352	IF ON SKIN: Wash with plenty of water
P304+P340	IF INHALED: Remove person to fresh air and keep comfortable for breathing
P311	call a POISON CENTER/doctor
P321	specific treatment (see on this label)
P330	rinse mouth
P361+P364	take off immediately all contaminated clothing and wash it before reuse
P370+P378	in case of fire: Use sand, carbon dioxide or powder extinguisher 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

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Precautionary statements	
P501	dispose of contents/container in accordance with local/regional/national/international regulations

2.3 Other hazards

This material is combustible, but will not ignite readily.

Results of PBT and vPvB assessment

According to the results of its assessment, this substance is not a PBT or a vPvB.

Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of $\geq 0,1\%$.

SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance	Nitrobenzene-d5
Identifiers	
CAS No	4165-60-0
Purity	>98 %
Molecular formula	C6D5NO2
Molar mass	128 g/mol

SECTION 4: First aid measures

4.1 Description of first aid measures

General notes

Do not leave affected person unattended. Remove victim out of the danger area. Keep affected person warm, still and covered. Take off immediately all contaminated clothing. In all cases of doubt, or when symptoms persist, seek medical advice. In case of unconsciousness place person in the recovery position. Never give anything by mouth.

Following inhalation

If breathing is irregular or stopped, immediately seek medical assistance and start first aid actions. Provide fresh air.

Following skin contact

Wash with plenty of soap and water.

Following eye contact

Remove contact lenses, if present and easy to do. Continue rinsing. Irrigate copiously with clean, fresh water for at least 10 minutes, holding the eyelids apart.

Following ingestion

Rinse mouth with water (only if the person is conscious). Do NOT induce vomiting.

4.2 Most important symptoms and effects, both acute and delayed

Symptoms and effects are not known to date.

4.3 Indication of any immediate medical attention and special treatment needed

none

SECTION 5: Firefighting measures

5.1 Extinguishing media

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Suitable extinguishing media

Water spray, Alcohol resistant foam, BC-powder, Carbon dioxide (CO₂)

Unsuitable extinguishing media

Water jet

5.2 Special hazards arising from the substance or mixture

In case of insufficient ventilation and/or in use, may form flammable/explosive vapour-air mixture. Solvent vapours are heavier than air and may spread along floors. Places which are not ventilated, e.g. unventilated below ground level areas such as trenches, conduits and shafts, are particularly prone to the presence of flammable substances or mixtures.

Hazardous combustion products

Nitrogen oxides (NO_x), Carbon monoxide (CO), Carbon dioxide (CO₂)

5.3 Advice for firefighters

In case of fire and/or explosion do not breathe fumes. Co-ordinate firefighting measures to the fire surroundings. Do not allow firefighting water to enter drains or water courses. Collect contaminated firefighting water separately. Fight fire with normal precautions from a reasonable distance.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

For non-emergency personnel

Remove persons to safety.

For emergency responders

Wear breathing apparatus if exposed to vapours/dust/spray/gases.

6.2 Environmental precautions

Keep away from drains, surface and ground water. Retain contaminated washing water and dispose of it. If substance has entered a water course or sewer, inform the responsible authority.

6.3 Methods and material for containment and cleaning up

Advice on how to contain a spill

Covering of drains

Advice on how to clean up a spill

Wipe up with absorbent material (e.g. cloth, fleece). Collect spillage: sawdust, kieselgur (diatomite), sand, universal binder

Appropriate containment techniques

Use of adsorbent materials.

Other information relating to spills and releases

Place in appropriate containers for disposal. Ventilate affected area.

6.4 Reference to other sections

Hazardous combustion products: see section 5. Personal protective equipment: see section 8. Incompatible materials: see section 10. Disposal considerations: see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Recommendations

Store in a dry place.

- Measures to prevent fire as well as aerosol and dust generation

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Use local and general ventilation. Avoidance of ignition sources. Keep away from sources of ignition - No smoking. Take precautionary measures against static discharge. Use only in well-ventilated areas. Due to danger of explosion, prevent leakage of vapours into cellars, flues and ditches. Ground/bond container and receiving equipment. Use explosion-proof electrical/ventilating/lighting/equipment. Use only non-sparking tools.

- Specific notes/details

Places which are not ventilated, e.g. unventilated below ground level areas such as trenches, conduits and shafts, are particularly prone to the presence of flammable substances or mixtures. Vapours are heavier than air, spread along floors and form explosive mixtures with air. Vapours may form explosive mixtures with air.

Advice on general occupational hygiene

Wash hands after use. Do not eat, drink and smoke in work areas. Remove contaminated clothing and protective equipment before entering eating areas. Never keep food or drink in the vicinity of chemicals. Never place chemicals in containers that are normally used for food or drink. Keep away from food, drink and animal feedingstuffs.

7.2 Conditions for safe storage, including any incompatibilities

Managing of associated risks

- Explosive atmospheres

Keep container tightly closed and in a well-ventilated place. Use local and general ventilation. Keep cool. Protect from sunlight.

- Flammability hazards

Keep away from sources of ignition - No smoking. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Take precautionary measures against static discharge. Protect from sunlight.

- Ventilation requirements

Keep any substance that emits harmful vapours or gases in a place that allows these to be permanently extracted. Use local and general ventilation. Ground/bond container and receiving equipment.

- Specific designs for storage rooms or vessels

- Storage temperature

Recommended storage temperature: 15 – 20 °C
15 °C

- Packaging compatibilities

Only packagings which are approved (e.g. acc. to the Dangerous Goods Regulations) may be used.

7.3 Specific end use(s)

See section 16 for a general overview.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Occupational exposure limit values (Workplace Exposure Limits)											
Country	Name of agent	CAS No	Identifier	TWA [ppm]	TWA [mg/m³]	STEL [ppm]	STEL [mg/m³]	Ceiling-C [ppm]	Ceiling-C [mg/m³]	Notation	Source
CN	nitrobenzene	98-95-3	OEL		2					H	GBZ 2.1

Notation

Ceiling-C ceiling value is a limit value above which exposure should not occur

H absorbed through the skin

STEL short-term exposure limit: a limit value above which exposure should not occur and which is related to a 15-minute period (unless otherwise specified)

TWA time-weighted average (long-term exposure limit): measured or calculated in relation to a reference period of 8 hours
time-weighted average (unless otherwise specified)

8.2 Exposure controls

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Appropriate engineering controls

General ventilation.

Individual protection measures (personal protective equipment)

Eye/face protection

Wear eye/face protection.

Skin protection

- Hand protection

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374. Check leak-tightness/impermeability prior to use. In the case of wanting to use the gloves again, clean them before taking off and air them well. For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves.

- Type of material

Nitrile

IIR: isobutene-isoprene (butyl) rubber

- Breakthrough times of the glove material

>30 minutes (permeation: level 2)

- Other protection measures

Take recovery periods for skin regeneration. Preventive skin protection (barrier creams/ointments) is recommended. Wash hands thoroughly after handling.

Respiratory protection

In case of inadequate ventilation wear respiratory protection.

Environmental exposure controls

Use appropriate container to avoid environmental contamination. Keep away from drains, surface and ground water.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Appearance

Physical state	liquid
Colour	not determined
Particle	not relevant (liquid)
Odour	pungent

Other safety parameters

pH (value)	not determined
Melting point/freezing point	5.26 °C
Initial boiling point and boiling range	211 °C at 1,013 hPa
Flash point	88 °C at 1,013 hPa (closed cup)
Evaporation rate	not determined

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Flammability (solid, gas)	not relevant, (fluid)
Vapour pressure	20 Pa at 20 °C
Density	1.25 g/cm³ at 25 °C
Vapour density	this information is not available

Solubility(ies)

- Water solubility	1.9 g/l at 20 °C
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Partition coefficient

- n-octanol/water (log KOW)	1.86 (pH value: 7.9, 24.5 °C) (ECHA)
- Soil organic carbon/water (log KOC)	2.07 (ECHA)
Auto-ignition temperature	480 °C at 1,013 hPa (ECHA) (auto-ignition temperature (liquids and gases))

Viscosity

- Dynamic viscosity	2.03 mPa s at 20 °C
Explosive properties	none
Oxidising properties	none

9.2 Other information

Refractive index	1.55 (20 °C) ((lit.))
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SECTION 10: Stability and reactivity

10.1 Reactivity

Concerning incompatibility: see below "Conditions to avoid" and "Incompatible materials". It's a reactive substance. The mixture contains reactive substance(s). Risk of ignition.

If heated:

Risk of ignition

10.2 Chemical stability

See below "Conditions to avoid".

10.3 Possibility of hazardous reactions

No known hazardous reactions.

10.4 Conditions to avoid

Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

Hints to prevent fire or explosion

Use explosion-proof electrical/ventilating/lighting/equipment. Use only non-sparking tools. Take precautionary measures against static discharge.

10.5 Incompatible materials

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Oxidisers

10.6 Hazardous decomposition products

Reasonably anticipated hazardous decomposition products produced as a result of use, storage, spill and heating are not known. Hazardous combustion products: see section 5.

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Classification acc. to GHS

Acute toxicity

Harmful if swallowed. Toxic in contact with skin. Toxic if inhaled.

- Acute toxicity estimate (ATE)

Oral	588 mg/kg
Dermal	760 mg/kg
Inhalation: vapour	3 mg/l/4h

Skin corrosion/irritation

Shall not be classified as corrosive/irritant to skin.

Serious eye damage/eye irritation

Shall not be classified as seriously damaging to the eye or eye irritant.

Respiratory or skin sensitisation

Shall not be classified as a respiratory or skin sensitiser.

Germ cell mutagenicity

Shall not be classified as germ cell mutagenic.

Carcinogenicity

Suspected of causing cancer.

Reproductive toxicity

May damage fertility.

Specific target organ toxicity - single exposure

Shall not be classified as a specific target organ toxicant (single exposure).

Specific target organ toxicity - repeated exposure

Causes damage to organs through prolonged or repeated exposure.

Aspiration hazard

Shall not be classified as presenting an aspiration hazard.

SECTION 12: Ecological information

12.1 Toxicity

Harmful to aquatic life with long lasting effects.

Aquatic toxicity (acute)			
Endpoint	Value	Species	Exposure time
LC50	92 mg/l	fish	96 h
EC50	35 mg/l	aquatic invertebrates	48 h
ErC50	18 mg/l	algae	96 h

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Aquatic toxicity (chronic)			
Endpoint	Value	Species	Exposure time
LC50	0.002 mg/l	fish	23 d

12.2 Persistence and degradability

Biodegradation

The substance is readily biodegradable.

Process of degradability		
Process	Degradation rate	Time
oxygen depletion	50 – 60 %	28 d

12.3 Bioaccumulative potential

Data are not available.

n-octanol/water (log KOW)	1.86 (pH value: 7.9, 24.5 °C) (ECHA)
BCF	3.1 (ECHA)

12.4 Mobility in soil

Henry's law constant	1.3 Pa m ³ /mol at 20 °C
The Organic Carbon normalised adsorption coefficient	2.07 (ECHA)

12.5 Results of PBT and vPvB assessment

According to the results of its assessment, this substance is not a PBT or a vPvB.

12.6 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of ≥ 0,1%.

12.7 Other adverse effects

Data are not available.

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Waste treatment-relevant information

Solvent reclamation/regeneration.

Sewage disposal-relevant information

Do not empty into drains. Avoid release to the environment. Refer to special instructions/safety data sheets.

Waste treatment of containers/packagings

Only packagings which are approved (e.g. acc. to the Dangerous Goods Regulations) may be used. Completely empty packages can be recycled. Handle contaminated packages in the same way as the substance itself.

Remarks

Please consider the relevant national or regional provisions. Waste shall be separated into the categories that can be

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handled separately by the local or national waste management facilities.

SECTION 14: Transport information

14.1 UN number

UN RTDG	UN 1662
IMDG-Code	UN 1662
ICAO-TI	UN 1662

14.2 UN proper shipping name

UN RTDG	NITROBENZENE
IMDG-Code	NITROBENZENE
ICAO-TI	Nitrobenzene

14.3 Transport hazard class(es)

UN RTDG	6.1
IMDG-Code	6.1
ICAO-TI	6.1

14.4 Packing group

UN RTDG	II
IMDG-Code	II
ICAO-TI	II

14.5 Environmental hazards

non-environmentally hazardous acc. to the dangerous goods regulations

14.6 Special precautions for user

There is no additional information.

14.7 Transport in bulk according to IMO instruments

The cargo is not intended to be carried in bulk.

Information for each of the UN Model Regulations

Transport information - National regulations - Additional information (UN RTDG)

UN number	1662
Class	6.1
Packing group	II
Danger label(s)	6.1



Special provisions (SP)	279 (UN RTDG)
Excepted quantities (EQ)	E4 (UN RTDG)

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Limited quantities (LQ) 100 ml (UN RTDG)

International Maritime Dangerous Goods Code (IMDG) - Additional information

Marine pollutant -
Danger label(s) 6.1



Special provisions (SP) 279
Excepted quantities (EQ) E4
Limited quantities (LQ) 100 mL
EmS F-A, S-A
Stowage category A

International Civil Aviation Organization (ICAO-IATA/DGR) - Additional information

Danger label(s) 6.1



Special provisions (SP) A113
Excepted quantities (EQ) E4
Limited quantities (LQ) 1 L

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

There is no additional information.

National inventories

Country	Inventory	Status
EU	REACH Reg.	substance is listed
US	TSCA	substance is listed (ACTIVE)

Legend

REACH Reg. REACH registered substances
TSCA Toxic Substance Control Act

15.2 Chemical Safety Assessment

No Chemical Safety Assessment has been carried out for this substance.

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SECTION 16: Other information

Indication of changes (revised safety data sheet)

Section	Former entry (text/value)	Actual entry (text/value)	Safety-relevant
1.3	Details of the supplier of the safety data sheet: Zeochem AG Joweid 5, CH-8630 Rüti Switzerland Telephone: +41 44 922 93 93 e-Mail: info@zeochem.com / info@zeochem.ch Website: https://www.zeochem.com	Details of the supplier of the safety data sheet: Zeochem AG Joweid 5, CH-8630 Rüti Switzerland Telephone: +41 44 922 93 93 e-Mail: info@zeochem.com Website: https://www.zeochem.com	yes
1.4		Poison centre: change in the listing (table)	yes
2.3		Endocrine disrupting properties: Does not contain an endocrine disruptor (ED) at a concentration of $\geq 0,1\%$.	yes
7.2		- Specific designs for storage rooms or vessels	yes
7.2		Storage temperature: Recommended storage temperature: 15 – 20 °C 15 °C	yes
8.1		Occupational exposure limit values (Workplace Exposure Limits): change in the listing (table)	yes
12.5	Results of PBT and vPvB assessment: Data are not available.	Results of PBT and vPvB assessment: According to the results of its assessment, this substance is not a PBT or a vPvB.	yes
12.6	Endocrine disrupting properties: Not listed.	Endocrine disrupting properties: Does not contain an endocrine disruptor (ED) at a concentration of $\geq 0,1\%$.	yes
15.1		National inventories: change in the listing (table)	yes

Key literature references and sources for data

General Rule for Classification and Hazard Communication of Chemicals (National Standard GB 13690). National Standard: Safety Data Sheet for Chemical Products - Content and Order of Sections. GB/T 16483. National Standard: Guidance on Compilation of Safety Data Sheet for Chemical Products. GB/T 17519.
UN Recommendations on the Transport of Dangerous Good. International Maritime Dangerous Goods Code (IMDG). Dangerous Goods Regulations (DGR) for the air transport (IATA).

List of relevant phrases (code and full text as stated in section 2 and 3)

Code	Text
H227	Combustible liquid.
H302	Harmful if swallowed.
H311	Toxic in contact with skin.
H331	Toxic if inhaled.
H351	Suspected of causing cancer.

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Code	Text
H360F	May damage fertility.
H372	Causes damage to organs through prolonged or repeated exposure.
H402	Harmful to aquatic life.
H412	Harmful to aquatic life with long lasting effects.

Disclaimer

This information is based upon the present state of our knowledge. This SDS has been compiled and is solely intended for this product.