Safety Data Sheet

Nitrobenzene-d5

According to Regulation (EC) No. 1907/2006 (REACH)

Classification acc. to 29 CFR 1910.1200

Version number: GHS 2.0
Replaces version of: 2022-03-23 (GHS 1)

Revision: 2023-02-02

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($^2H_5$)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 / info@zeochem.ch
Website: https://www.zeochem.com

1.4 Emergency telephone number

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
3.1O	acute toxicity (oral)	3	Acute Tox. 3	H301
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
4.1C	hazardous to the aquatic environment - chronic hazard	3	Aquatic Chronic 3	H412

For full text of abbreviations: see SECTION 16.

The most important adverse physicochemical, human health and environmental effects

Delayed or immediate effects can be expected after short or long-term exposure. Spillage and fire water can cause pollution of watercourses.

2.2 Label elements

Labelling

- Signal word danger

2.2.1.2 Pictograms

GHS06, GHS08	

Hazard statements	
H301+H311+H331	toxic if swallowed, in contact with skin or if inhaled
H351	suspected of causing cancer
H360F	may damage fertility
H372	causes damage to organs (blood) through prolonged or repeated exposure
H412	harmful to aquatic life with long lasting effects

Precautionary statements	
P201	obtain special instructions before use
P260	do not breathe dust/fume/gas/mist/vapours/spray
P273	avoid release to the environment
P280	wear protective gloves/protective clothing/eye protection/face protection/hearing protection
P301+P310	IF SWALLOWED: Immediately call a POISON CENTER/doctor
P304+P340	IF INHALED: Remove person to fresh air and keep comfortable for breathing
P311	call a POISON CENTER/doctor
P361+P364	take off immediately all contaminated clothing and wash it before reuse
P403+P233	store in a well-ventilated place. Keep container tightly closed
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.

SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance	Nitrobenzene-d5
Identifiers	
CAS No	4165-60-0
EC No	224-014-3

Purity >98 %

Specific Conc. Limits	M-Factors	ATE	Exposure route
-	-	100 $^{mg}/_{kg}$ 760 $^{mg}/_{kg}$ 3 $^{mg}/_{l}$/4h	oral dermal inhalation: vapour

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

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

Hazardous combustion products

Nitrogen oxides (NOx), 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.

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

Use local and general ventilation. Use only in well-ventilated areas.

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

- Ventilation requirements

Keep any substance that emits harmful vapours or gases in a place that allows these to be permanently extracted.

- Packaging compatibilities

Only packagings which are approved (e.g. acc. to ADR) 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
EU	nitrobenzene	98-95-3	IOELV	0.2	1					H	2022/431/EU
GB	nitrobenzene	98-95-3	WEL	0.2	1						EH40/2005

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

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

Physical state	liquid
Colour	not determined
Odour	pungent
Melting point/freezing point	5.26 °C
Boiling point or initial boiling point and boiling range	211 °C at 1,013 hPa
Flammability	this material is combustible, but will not ignite readily
Lower and upper explosion limit	not determined
Flash point	88 °C at 1,013 hPa (closed cup)
Auto-ignition temperature	480 °C at 1,013 hPa (ECHA) (auto-ignition temperature (liquids and gases))
Decomposition temperature	not relevant
pH (value)	not determined
Kinematic viscosity	not determined

Solubility(ies)

Water solubility	1.9 $^{g}/_{l}$ at 20 °C

Partition coefficient

Partition coefficient n-octanol/water (log value)	1.86 (pH value: 7.9, 24.5 °C) (ECHA)
Soil organic carbon/water (log KOC)	2.07 (ECHA)

Vapour pressure	20 Pa at 20 °C

Density and/or relative density

Density	1.25 $^{g}/_{cm^3}$ at 25 °C
Relative vapour density	information on this property is not available

Particle characteristics	not relevant (liquid)

9.2 Other information

Information with regard to physical hazard classes	hazard classes acc. to GHS (physical hazards): not relevant

Other safety characteristics

Refractive index	1.55 (20 °C) ((lit.))

SECTION 10: Stability and reactivity

10.1 Reactivity

Concerning incompatibility: see below "Conditions to avoid" and "Incompatible materials".

10.2 Chemical stability

See below "Conditions to avoid".

10.3 Possibility of hazardous reactions

No known hazardous reactions.

10.4 Conditions to avoid

There are no specific conditions known which have to be avoided.

10.5 Incompatible materials

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

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

- Acute toxicity estimate (ATE)

Oral	100 $^{mg}/_{kg}$
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 (blood) through prolonged or repeated exposure.

Hazard category	Target organ	Exposure route
1	blood	if exposed

Aspiration hazard

Shall not be classified as presenting an aspiration hazard.

11.2 Information on other hazards

There is no additional information.

SECTION 12: Ecological information

12.1 Toxicity

Harmful to aquatic life with long lasting effects.

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

Data are not available.

12.6 Endocrine disrupting properties

Not listed.

12.7 Other adverse effects

Data are not available.

SECTION 13: Disposal considerations

13.1 Waste treatment methods

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

It is a dangerous waste; only packagings which are approved (e.g. acc. to ADR) may be used. Completely emptied 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 handled separately by the local or national waste management facilities.

SECTION 14: Transport information

14.1 UN number or ID number

ADR/RID	UN 1662
IMDG-Code	UN 1662
ICAO-TI	UN 1662

14.2 UN proper shipping name

ADR/RID	NITROBENZENE
IMDG-Code	NITROBENZENE
ICAO-TI	Nitrobenzene

14.3 Transport hazard class(es)

ADR/RID	6.1
IMDG-Code	6.1
ICAO-TI	6.1

14.4 Packing group

ADR/RID	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

Provisions for dangerous goods (ADR) should be complied within the premises.

14.7 Maritime 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

Agreement concerning the International Carriage of Dangerous Goods by Road (ADR) - Additional information

Classification code	T1
Danger label(s)	6.1

Special provisions (SP)	279, 802(ADN)
Excepted quantities (EQ)	E4
Limited quantities (LQ)	100 ml
Transport category (TC)	2
Tunnel restriction code (TRC)	D/E
Hazard identification No	60
Emergency Action Code	2X

Regulations concerning the International Carriage of Dangerous Goods by Rail (RID) - Additional information

Classification code	T1
Danger label(s)	6.1

Special provisions (SP)	279, 802(ADN)
Excepted quantities (EQ)	E4
Limited quantities (LQ)	100 ml
Transport category (TC)	2
Hazard identification No	60

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

Relevant provisions of the European Union (EU)

Directive on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS)

not listed

Regulation concerning the establishment of a European Pollutant Release and Transfer Register (PRTR)

not listed

Water Framework Directive (WFD)

List of pollutants (WFD)

Name of substance	CAS No	Listed in	Remarks
Nitrobenzene-d5		a)	

Legend
A) Indicative list of the main pollutants

Regulation on persistent organic pollutants (POP)

Not listed.

National regulations (GB)

List of substances subject to authorisation (GB REACH, Annex 14) / SVHC - candidate list

Substance of Very High Concern (SVHC) acc. to GB REACH and HSE

Name of substance	CAS No	Listed in	Remarks
Nitrobenzene-d5	98-95-3	Candidate list	Repr. A57c

Legend
candidate list Substances meeting the criteria referred to in Article 57 and for eventual inclusion in Annex XIV
Repr. A57c Toxic for reproduction (Article 57c)

Restrictions according to GB REACH, Annex 17

Dangerous substances with restrictions (GB REACH, Annex 17)			
Name of substance	**Name acc. to inventory**	**CAS No**	**No**
Nitrobenzene-d5	this product meets the criteria for classification in accordance with Regulation No 1272/2008/EC		3
Nitrobenzene-d5	toxic for reproduction		30

National inventories

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

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.

SECTION 16: Other information

Indication of changes (revised safety data sheet)

Section	Former entry (text/value)	Actual entry (text/value)	Safety-relevant
1.1	Registration number (REACH): this information is not available		yes
1.4		Poison centre: change in the listing (table)	yes
8.1		Occupational exposure limit values (Workplace Exposure Limits): change in the listing (table)	yes
9.2	Temperature class (EU, acc. to ATEX): T1 (maximum permissible surface temperature on the equipment: 450°C)		yes
14.7	Classification code: 6.1	Classification code: T1	yes
15.1	Restrictions according to REACH, Annex XVII		yes
15.1		Dangerous substances with restrictions (REACH, Annex XVII): change in the listing (table)	yes

Section	Former entry (text/value)	Actual entry (text/value)	Safety-relevant
15.1	List of substances subject to authorisation (REACH, Annex XIV) / SVHC - candidate list		yes
15.1		Substance of Very High Concern (SVHC): change in the listing (table)	yes
15.1		National regulations (GB)	yes
15.1		List of substances subject to authorisation (GB REACH, Annex 14) / SVHC - candidate list	yes
15.1		Substance of Very High Concern (SVHC) acc. to GB REACH and HSE: change in the listing (table)	yes
15.1		Restrictions according to GB REACH, Annex 17	yes
15.1		Dangerous substances with restrictions (GB REACH, Annex 17): change in the listing (table)	yes
16	Key literature references and sources for data: Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures. Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU.Agreement concerning the International Carriage of Dangerous Goods by Road (ADR). Regulations concerning the International Carriage of Dangerous Goods by Rail (RID). International Maritime Dangerous Goods Code (IMDG). Dangerous Goods Regulations (DGR) for the air transport (IATA).	Key literature references and sources for data: Agreement concerning the International Carriage of Dangerous Goods by Road (ADR). Regulations concerning the International Carriage of Dangerous Goods by Rail (RID). International Maritime Dangerous Goods Code (IMDG). Dangerous Goods Regulations (DGR) for the air transport (IATA).	yes

Key literature references and sources for data

Agreement concerning the International Carriage of Dangerous Goods by Road (ADR). Regulations concerning the International Carriage of Dangerous Goods by Rail (RID). 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
H301	Toxic if swallowed.
H311	Toxic in contact with skin.
H331	Toxic if inhaled.
H351	Suspected of causing cancer.
H360F	May damage fertility.
H372	Causes damage to organs (blood) through prolonged or repeated exposure.
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.