

# Safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU



## 3-Nitroaniline 99%, for synthesis

article number: **9867**  
Version: **3.0 en**  
Replaces version of: 12.01.2022  
Version: (2)

date of compilation: 29.07.2016  
Revision: 02.03.2024

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

### 1.1 Product identifier

Identification of the substance	<b>3-Nitroaniline</b> 99%, for synthesis
Article number	9867
Registration number (REACH)	It is not required to list the identified uses because the substance is not subject to registration according to REACH (< 1 t/a).
Index number in CLP Annex VI	612-012-00-9
EC number	202-729-1
CAS number	99-09-2

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

Relevant identified uses:	Laboratory chemical Laboratory and analytical use
Uses advised against:	Do not use for products which come into contact with foodstuffs. Do not use for private purposes (household). Food, drink and animal feeding-stuffs.

### 1.3 Details of the supplier of the safety data sheet

Carl Roth GmbH + Co. KG  
Schoemperlenstr. 3-5  
D-76185 Karlsruhe  
Germany

**Telephone:** +49 (0) 721 - 56 06 0  
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**e-mail:** [sicherheit@carlroth.de](mailto:sicherheit@carlroth.de)  
**Website:** [www.carlroth.de](http://www.carlroth.de)

Competent person responsible for the safety data sheet: Department Health, Safety and Environment

**e-mail (competent person):** [sicherheit@carlroth.de](mailto:sicherheit@carlroth.de)

### 1.4 Emergency telephone number

## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008 (CLP)

Section	Hazard class	Cat-egory	Hazard class and category	Hazard statement
3.10	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

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Section	Hazard class	Cat-egory	Hazard class and category	Hazard statement
3.9	Specific target organ toxicity - repeated exposure	2	STOT RE 2	H373
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 according to Regulation (EC) No 1272/2008 (CLP)

#### Signal word

**Danger**

#### Pictograms

GHS06, GHS08



#### Hazard statements

H301+H311+H331 Toxic if swallowed, in contact with skin or if inhaled  
H373 May cause damage to organs through prolonged or repeated exposure  
H412 Harmful to aquatic life with long lasting effects

#### Precautionary statements

##### Precautionary statements - prevention

P280 Wear protective clothing/eye protection/face protection

##### Precautionary statements - response

P301+P310 IF SWALLOWED: Immediately call a POISON CENTER/doctor  
P302+P352 IF ON SKIN: Wash with plenty of water  
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing  
P312 Call a POISON CENTRE/doctor if you feel unwell

#### Labelling of packages where the contents do not exceed 125 ml

Signal word: **Danger**

Symbol(s)



H301+H311+H331 Toxic if swallowed, in contact with skin or if inhaled.  
H412 Harmful to aquatic life with long lasting effects.

P280 Wear protective clothing/eye protection/face protection.  
P301+P310 IF SWALLOWED: Immediately call a POISON CENTER/doctor.  
P302+P352 IF ON SKIN: Wash with plenty of water.  
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.  
P312 Call a POISON CENTRE/doctor if you feel unwell.

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### 2.3 Other hazards

#### 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	3-Nitroaniline
Molecular formula	$C_6H_6N_2O_2$
Molar mass	138,1 g/mol
CAS No	99-09-2
EC No	202-729-1
Index No	612-012-00-9

Substance, Specific Conc. Limits, M-factors, ATE			
Specific Conc. Limits	M-Factors	ATE	Exposure route
-	-	100 mg/kg 300 mg/kg >0,5 mg/l/4h	oral dermal inhalation: dust/ mist

## SECTION 4: First aid measures

### 4.1 Description of first aid measures



#### General notes

Take off immediately all contaminated clothing. Self-protection of the first aider.

#### Following inhalation

Call a physician immediately. If breathing is irregular or stopped, administer artificial respiration.

#### Following skin contact

After contact with skin, wash immediately with plenty of water.

#### Following eye contact

Rinse cautiously with water for several minutes. In all cases of doubt, or when symptoms persist, seek medical advice.

#### Following ingestion

Rinse mouth immediately and drink plenty of water. Call a physician immediately.

### 4.2 Most important symptoms and effects, both acute and delayed

Symptoms and effects are not known to date.

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### 4.3 Indication of any immediate medical attention and special treatment needed

none

## SECTION 5: Firefighting measures

### 5.1 Extinguishing media



#### Suitable extinguishing media

co-ordinate firefighting measures to the fire surroundings!  
water, foam, alcohol resistant foam, dry extinguishing powder, ABC-powder

#### Unsuitable extinguishing media

water jet

### 5.2 Special hazards arising from the substance or mixture

Combustible.

#### Hazardous combustion products

In case of fire may be liberated: Nitrogen oxides (NO<sub>x</sub>), Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>)

### 5.3 Advice for firefighters

In case of fire and/or explosion do not breathe fumes. Do not allow firefighting water to enter drains or water courses. Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus. Wear full chemical protective clothing.

## SECTION 6: Accidental release measures

### 6.1 Personal precautions, protective equipment and emergency procedures



#### For non-emergency personnel

Use personal protective equipment as required. Avoid contact with skin, eyes and clothes. Do not breathe dust.

### 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. Take up mechanically.

#### Advice on how to clean up a spill

Take up mechanically. Control of dust.

#### Other information relating to spills and releases

Place in appropriate containers for disposal. Ventilate affected area.

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### 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

Provision of sufficient ventilation. Use extractor hood (laboratory). Handle and open container with care. Avoid dust formation. Clear contaminated areas thoroughly.

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

Removal of dust deposits.

#### Advice on general occupational hygiene

When using do not eat or drink. Thorough skin-cleansing after handling the product.

### 7.2 Conditions for safe storage, including any incompatibilities

Store in a dry place.

#### Incompatible substances or mixtures

Observe hints for combined storage.

#### Consideration of other advice:

Store locked up.

#### 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.

#### Specific designs for storage rooms or vessels

Recommended storage temperature: 15 – 25 °C

### 7.3 Specific end use(s)

No information available.

## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### National limit values

#### Occupational exposure limit values (Workplace Exposure Limits)

This information is not available.

### 8.2 Exposure controls

#### Individual protection measures (personal protective equipment)

##### Eye/face protection



Use safety goggle with side protection.

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### 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. 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. The times are approximate values from measurements at 22 ° C and permanent contact. Increased temperatures due to heated substances, body heat etc. and a reduction of the effective layer thickness by stretching can lead to a considerable reduction of the breakthrough time. If in doubt, contact manufacturer. At an approx. 1.5 times larger / smaller layer thickness, the respective breakthrough time is doubled / halved. The data apply only to the pure substance. When transferred to substance mixtures, they may only be considered as a guide.

#### • type of material

NBR (Nitrile rubber)

#### • material thickness

>0,11 mm

#### • breakthrough times of the glove material

>480 minutes (permeation: level 6)

#### • other protection measures

Take recovery periods for skin regeneration. Preventive skin protection (barrier creams/ointments) is recommended.

### Respiratory protection



Respiratory protection necessary at: Dust formation. Particulate filter device (EN 143). P3 (filters at least 99,95 % of airborne particles, colour code: White).

### Environmental exposure controls

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	solid
Colour	yellow-orange
Odour	characteristic
Melting point/freezing point	109 – 112 °C
Boiling point or initial boiling point and boiling range	306 °C
Flammability	this material is combustible, but will not ignite readily
Lower and upper explosion limit	not determined

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Flash point	196 °C
Auto-ignition temperature	not determined
Decomposition temperature	247 °C at 1.013 hPa
pH (value)	not applicable
Kinematic viscosity	not relevant
<u>Solubility(ies)</u>	
Water solubility	1,25 g/l at 20 °C
<u>Partition coefficient</u>	
Partition coefficient n-octanol/water (log value):	1,37 (TOXNET)
Vapour pressure	1 hPa at 104 °C
<u>Density and/or relative density</u>	
Density	0,9 g/cm <sup>3</sup>
Relative vapour density	Information on this property is not available.
Particle characteristics	No data available.
<u>Other safety parameters</u>	
Oxidising properties	none
<b>9.2 Other information</b>	
Information with regard to physical hazard classes:	hazard classes acc. to GHS (physical hazards): not relevant
Other safety characteristics:	
Temperature class (EU, acc. to ATEX)	T1 Maximum permissible surface temperature on the equipment: 450°C

## SECTION 10: Stability and reactivity

### 10.1 Reactivity

The product in the delivered form is not dust explosion capable; the enrichment of fine dust however leads to the danger of dust explosion.

### 10.2 Chemical stability

The material is stable under normal ambient and anticipated storage and handling conditions of temperature and pressure.

### 10.3 Possibility of hazardous reactions

**Violent reaction with:** strong oxidiser, Alkali metals, Magnesium, Organic substances, Nitric acid, Sulphuric acid, Water

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### 10.4 Conditions to avoid

Keep away from heat. Humidity. Decomposition takes place from temperatures above: 247 °C at 1.013 hPa.

### 10.5 Incompatible materials

There is no additional information.

### 10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

## SECTION 11: Toxicological information

### 11.1 Information on hazard classes as defined in Regulation (EC) No 1272/2008

#### Classification according to GHS (1272/2008/EC, CLP)

##### Acute toxicity

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

##### 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

Shall not be classified as carcinogenic.

##### Reproductive toxicity

Shall not be classified as a reproductive toxicant.

##### Specific target organ toxicity - single exposure

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

##### Specific target organ toxicity - repeated exposure

May cause damage to organs through prolonged or repeated exposure.

##### Aspiration hazard

Shall not be classified as presenting an aspiration hazard.

#### Symptoms related to the physical, chemical and toxicological characteristics

##### • If swallowed

Data are not available.

##### • If in eyes

Data are not available.

##### • If inhaled

Data are not available.

##### • If on skin

Data are not available.



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### • Other information

This information is based upon the present state of our knowledge.

### 11.2 Endocrine disrupting properties

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

### 11.3 Information on other hazards

There is no additional information.

## SECTION 12: Ecological information

### 12.1 Toxicity

Harmful to aquatic life with long lasting effects.

### 12.2 Persistence and degradability

Theoretical Oxygen Demand (without nitrification): 1,158 mg/mg

Theoretical Oxygen Demand (with nitrification): 1,651 mg/mg

Theoretical Carbon Dioxide: 1,912 mg/mg

### 12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW)	1,37 (TOXNET)
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### 12.4 Mobility in soil

Data are not available.

### 12.5 Results of PBT and vPvB assessment

Data are not available.

### 12.6 Endocrine disrupting properties

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

### 12.7 Other adverse effects

Data are not available.

## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods



This material and its container must be disposed of as hazardous waste. Dispose of contents/container in accordance with local/regional/national/international regulations.

#### 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. Handle contaminated packages in the same way as the substance itself. Completely emptied packages can be recycled.

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### 13.2 Relevant provisions relating to waste

The allocation of waste identity numbers/waste descriptions must be carried out according to the EEC, specific to the industry and process.

#### Properties of waste which render it hazardous

**HP 5** specific target organ toxicity (STOT)/aspiration toxicity

**HP 6** acute toxicity

**HP 14** ecotoxic

### 13.3 Remarks

Waste shall be separated into the categories that can be handled separately by the local or national waste management facilities. Please consider the relevant national or regional provisions. Non-contaminated packages may be recycled.

## SECTION 14: Transport information

### 14.1 UN number or ID number

ADR	UN 1661
IMDG-Code	UN 1661
ICAO-TI	UN 1661

### 14.2 UN proper shipping name

ADR	NITROANILINES
IMDG-Code	NITROANILINES
ICAO-TI	Nitroanilines

### 14.3 Transport hazard class(es)

ADR	6.1
IMDG-Code	6.1
ICAO-TI	6.1

### 14.4 Packing group

ADR	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.

### 14.8 Information for each of the UN Model Regulations

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

Proper shipping name	NITROANILINES
Particulars in the transport document	UN1661, NITROANILINES, 6.1, II, (D/E)
Classification code	T2
Danger label(s)	6.1
Special provisions (SP)	279, 802(ADN)
Excepted quantities (EQ)	E4
Limited quantities (LQ)	500 g
Transport category (TC)	2
Tunnel restriction code (TRC)	D/E
Hazard identification No	60

### International Maritime Dangerous Goods Code (IMDG) - Additional information

Proper shipping name	NITROANILINES
Particulars in the shipper's declaration	UN1661, NITROANILINES, 6.1, II
Marine pollutant	-
Danger label(s)	6.1
Special provisions (SP)	279
Excepted quantities (EQ)	E4
Limited quantities (LQ)	500 g
EmS	F-A, S-A
Stowage category	A

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

Proper shipping name	Nitroanilines
Particulars in the shipper's declaration	UN1661, Nitroanilines, 6.1, II
Danger label(s)	6.1
Special provisions (SP)	A113
Excepted quantities (EQ)	E4
Limited quantities (LQ)	1 kg



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### Regulation on drug precursors

not listed

### Regulation on substances that deplete the ozone layer (ODS)

not listed

### Regulation concerning the export and import of hazardous chemicals (PIC)

not listed

### Regulation on persistent organic pollutants (POP)

not listed

### Other information

Directive 94/33/EC on the protection of young people at work. Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.

### National inventories

Country	Inventory	Status
AU	AIIC	substance is listed
CA	DSL	substance is listed
CN	IECSC	substance is listed
EU	ECSI	substance is listed
EU	REACH Reg.	substance is listed
JP	CSCL-ENCS	substance is listed
KR	KECI	substance is listed
MX	INSQ	substance is listed
NZ	NZIoC	substance is listed
PH	PICCS	substance is listed
TW	TCSI	substance is listed
US	TSCA	substance is listed (ACTIVE)
VN	NCI	substance is listed

#### Legend

AIIC	Australian Inventory of Industrial Chemicals
CSCL-ENCS	List of Existing and New Chemical Substances (CSCL-ENCS)
DSL	Domestic Substances List (DSL)
ECSI	EC Substance Inventory (EINECS, ELINCS, NLP)
IECSC	Inventory of Existing Chemical Substances Produced or Imported in China
INSQ	National Inventory of Chemical Substances
KECI	Korea Existing Chemicals Inventory
NCI	National Chemical Inventory
NZIoC	New Zealand Inventory of Chemicals
PICCS	Philippine Inventory of Chemicals and Chemical Substances (PICCS)
REACH Reg.	REACH registered substances
TCSI	Taiwan Chemical Substance Inventory
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
2.3		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

#### Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
ADR	Accord relatif au transport international des marchandises dangereuses par route (Agreement concerning the International Carriage of Dangerous Goods by Road)
ATE	Acute Toxicity Estimate
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
CLP	Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures
DGR	Dangerous Goods Regulations (see IATA/DGR)
EC No	The EC Inventory (EINECS, ELINCS and the NLP-list) is the source for the seven-digit EC number, an identifier of substances commercially available within the EU (European Union)
ED	Endocrine disruptor
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
EmS	Emergency Schedule
GHS	"Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Nations
IATA	International Air Transport Association
IATA/DGR	Dangerous Goods Regulations (DGR) for the air transport (IATA)
ICAO	International Civil Aviation Organization
ICAO-TI	Technical instructions for the safe transport of dangerous goods by air
IMDG	International Maritime Dangerous Goods Code
IMDG-Code	International Maritime Dangerous Goods Code
index No	The Index number is the identification code given to the substance in Part 3 of Annex VI to Regulation (EC) No 1272/2008
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SVHC	Substance of Very High Concern
VOC	Volatile Organic Compounds
vPvB	Very Persistent and very Bioaccumulative

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### 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). 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.
H373	May cause damage to organs 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.