

# safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU



## 4-nitroaniline 98,5%, for synthesis

article number: **9850**  
Version: **1.0 en**

date of compilation: 2016-07-26

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

### 1.1 Product identifier

Identification of the substance	<b>4-nitroaniline</b>
Article number	9850
Registration number (REACH)	01-2119942160-50-xxxx
Index No	612-012-00-9
EC number	202-810-1
CAS number	100-01-6

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

**Identified uses:**

### 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

**Telefax:** +49 (0) 721 - 56 06 149

**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

Emergency information service **Poison Centre Munich: +49/(0)89 19240**

## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

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

Classification acc. to GHS			
Section	Hazard class	Hazard class and category	Hazard statement
3.1O	acute toxicity (oral)	(Acute Tox. 3)	H301
3.1D	acute toxicity (dermal)	(Acute Tox. 3)	H311
3.1I	acute toxicity (inhal.)	(Acute Tox. 3)	H331
3.9	specific target organ toxicity - repeated exposure	(STOT RE 2)	H373
4.1C	hazardous to the aquatic environment - chronic hazard	(Aquatic Chronic 3)	H412

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### Remarks

For full text of Hazard- and EU Hazard-statements: see SECTION 16.

## 2.2 Label elements

### Labelling according to Regulation (EC) No 1272/2008 (CLP)

#### Signal word

**Danger**

#### Pictograms



#### 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 CENTER/doctor/.../if you feel unwell.

##### Precautionary statements - storage

P405 Store locked up.

##### Precautionary statements - disposal

P501 Dispose of contents/container to ...

#### 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/physician.  
P302+P352 IF ON SKIN: Wash with plenty of water.  
P304+P340 IF INHALED: Remove person to fresh air and keep at rest in a position comfortable for breathing.  
P312 Call a POISON CENTER/doctor if you feel unwell.  
P501 Dispose of contents/container to industrial combustion plant.

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### 2.3 Other hazards

There is no additional information.

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Name of substance	4-nitroaniline
Index No	612-012-00-9
Registration number (REACH)	01-2119942160-50-xxxx
EC number	202-810-1
CAS number	100-01-6
Molecular formula	C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>
Molar mass	138,1 g/mol

## 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

After eye contact: Causes tears, Conjunctival redness of the eyes,

Following skin contact: Localised redness,

After ingestion: Abdominal pain, Gastrointestinal complaints, Nausea, Vomiting,

Following inhalation: Cough, pain, choking, and breathing difficulties

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

none

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### SECTION 5: Firefighting measures

#### 5.1 Extinguishing media

##### Suitable extinguishing media

Co-ordinate fire-fighting measures to the fire surroundings  
water spray, foam, dry extinguishing powder, carbon dioxide (CO<sub>2</sub>)

##### Unsuitable extinguishing media

water jet

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

Combustible. Vapours are heavier than air, spread along floors and form explosive mixtures with air.

##### 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

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.

##### Special protective equipment for firefighters

Protective clothing against liquid and gaseous chemicals, including liquid aerosols and solid particles. Self-contained breathing apparatus (SCBA). Self-contained breathing apparatus (EN 133).

### SECTION 6: Accidental release measures

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

##### For non-emergency personnel

Wearing of suitable protective equipment (including personal protective equipment referred to under Section 8 of the safety data sheet) to prevent any contamination of skin, eyes and personal clothing. Avoid contact with skin, eyes and clothes.

#### 6.2 Environmental precautions

Keep away from drains, surface and ground water. Retain contaminated washing water and dispose it.

#### 6.3 Methods and material for containment and cleaning up

##### Advices on how to contain a spill

Covering of drains.

##### Advices 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.

##### 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.

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### 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.

- **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**

Use local and general ventilation.

#### 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)

Country	Name of agent	CAS No	Notation	Identifier	TWA [mg/m <sup>3</sup> ]	STEL [mg/m <sup>3</sup> ]	Source
IE	dusts non-specific		i	OELV	10		S.I. No. 619 of 2001
IE	dusts non-specific		r	OELV	4		S.I. No. 619 of 2001
IE	4-nitroaniline	100-01-6		OELV	3		S.I. No. 619 of 2001

##### Notation

i Inhalable fraction

r Respirable fraction

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

##### Relevant DNELs/DMELs/PNECs and other threshold levels

- **human health values**

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Endpoint	Threshold level	Protection goal, route of exposure	Used in	Exposure time
DNEL	0,201 mg/m <sup>3</sup>	human, inhalatory	worker (industry)	chronic - systemic effects
DNEL	0,176 mg/kg bw/day	human, dermal	worker (industry)	chronic - systemic effects

### • environmental values

Endpoint	Threshold level	Environmental compartment	Exposure time
PNEC	0,024 mg/l	freshwater	short-term (single instance)
PNEC	0,002 mg/l	marine water	short-term (single instance)
PNEC	0,24 mg/l	water	continuous
PNEC	1 mg/l	sewage treatment plant (STP)	short-term (single instance)
PNEC	64,25 mg/kg	freshwater sediment	short-term (single instance)
PNEC	64,25 mg/kg	marine sediment	short-term (single instance)
PNEC	25,96 mg/kg	soil	short-term (single instance)

## 8.2 Exposure controls

### Individual protection measures (personal protective equipment)



#### Eye/face protection

Use safety goggle with side 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. 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

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.

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### 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

#### Appearance

Physical state	solid (solid matter)
Colour	brown
Odour	this information is not available
Odour threshold	No data available

#### Other physical and chemical parameters

pH (value)	This information is not available.
Melting point/freezing point	158 °C at 975 hPa
Initial boiling point and boiling range	>800 °C at 975 hPa
Flash point	100,8 °C at 975 hPa
Evaporation rate	no data available
Flammability (solid, gas)	Non-flammable
<u>Explosive limits</u>	
• lower explosion limit (LEL)	this information is not available
• upper explosion limit (UEL)	this information is not available
Explosion limits of dust clouds	these information are not available
Vapour pressure	1,33 hPa at 142 °C
Density	0,951 g/cm <sup>3</sup> at 30 °C
Vapour density	4,77 (air = 1)
Bulk density	630 kg/m <sup>3</sup>
Relative density	Information on this property is not available.
<u>Solubility(ies)</u>	
Water solubility	1.000 mg/l at 30 °C
<u>Partition coefficient</u>	
n-octanol/water (log KOW)	1,2 (pH value: 4,71, 30 °C) (ECHA)
Soil organic carbon/water (log KOC)	2,038 (ECHA)
Auto-ignition temperature	500 °C
Decomposition temperature	no data available
Viscosity	not relevant (solid matter)
Explosive properties	shall not be classified as explosive

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Oxidising properties none

### 9.2 Other information

There is no additional information.

## 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: Acid chlorides, inorganic, Strong oxidiser, Strong acid, Acid halides

### 10.4 Conditions to avoid

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

### 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 toxicological effects

#### Acute toxicity

Exposure route	Endpoint	Value	Species	Source
oral	LD50	750 mg/kg	rat	
oral	LD50	75 mg/kg	bird	ECHA
dermal	LD50	>2.500 mg/kg	rabbit	
dermal	LD50	>500 mg/kg	guinea pig	ECHA

#### 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.

#### Summary of evaluation of the CMR properties

Shall not be classified as germ cell mutagenic, carcinogenic nor as a reproductive toxicant



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### • 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

abdominal pain, nausea, vomiting

#### • If in eyes

causes tears, slightly irritant

#### • If inhaled

cough, pain, choking, and breathing difficulties

#### • If on skin

localised redness

### Other information

None

## SECTION 12: Ecological information

### 12.1 Toxicity

Harmful to aquatic life with long lasting effects.

#### Aquatic toxicity (acute)

Endpoint	Value	Species	Source	Exposure time
LC50	87,6 mg/l	zebra fish (Danio rerio)	ECHA	96 h
EC50	17 mg/l	daphnia magna		48 h

#### Aquatic toxicity (chronic)

May cause long-term adverse effects in the aquatic environment.

Endpoint	Value	Species	Source	Exposure time
LC50	24 mg/l	aquatic invertebrates	ECHA	24 h
EC50	68 mg/l	algae	ECHA	24 h

### 12.2 Process of degradability

The substance is readily biodegradable.

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

Theoretical Oxygen Demand: 1,158 mg/mg

Theoretical Carbon Dioxide: 1,912 mg/mg

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Process	Degradation rate	Time
biotic/abiotic	>95 %	14 d

### 12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW)

1,2 (pH value: 4,71, 30 °C)

BCF

3,8 (3,8)

### 12.4 Mobility in soil

Henry's law constant

0,001 Pa m<sup>3</sup>/mol at 25 °C

The Organic Carbon normalised adsorption coefficient

2,038

### 12.5 Results of PBT and vPvB assessment

Data are not available.

### 12.6 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.

### 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.

### 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.

## SECTION 14: Transport information

14.1	UN number	1661
14.2	UN proper shipping name	NITROANILINES
	Hazardous ingredients	4-nitroaniline
14.3	Transport hazard class(es)	
	Class	6.1 (toxic substances)
14.4	Packing group	II (substance presenting medium danger)
14.5	Environmental hazards	none (non-environmentally hazardous acc. to the dangerous goods regulations)

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### 14.6 Special precautions for user

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

### 14.7 Transport in bulk according to Annex II of MARPOL and the IBC Code

The cargo is not intended to be carried in bulk.

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

#### • Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN)

UN number	1661
Proper shipping name	NITROANILINES
Particulars in the transport document	UN1661, NITROANILINES, 6.1, II, (D/E)
Class	6.1
Classification code	T2
Packing group	II
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)

UN number	1661
Proper shipping name	NITROANILINES
Particulars in the shipper's declaration	UN1661, NITROANILINES, 6.1, II
Class	6.1
Packing group	II
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

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### 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)

- **Regulation 649/2012/EU concerning the export and import of hazardous chemicals (PIC)**  
Not listed.

- **Regulation 1005/2009/EC on substances that deplete the ozone layer (ODS)**  
Not listed.

- **Regulation 850/2004/EC on persistent organic pollutants (POP)**  
Not listed.

- **Restrictions according to REACH, Annex XVII**  
not listed

- **List of substances subject to authorisation (REACH, Annex XIV)**  
not listed

- **Seveso Directive**

2012/18/EU (Seveso III)				
No	Dangerous substance/hazard categories	Qualifying quantity (tonnes) for the application of lower and upper-tier requirements		Notes
H2	acute toxic (cat. 2 + cat. 3, inhal.)	50	200	41)

##### Notation

41) - Category 2, all exposure routes  
- category 3, inhalation exposure route

**Directive 2011/65/EU on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS) - Annex II**

not listed

**Regulation 166/2006/EC concerning the establishment of a European Pollutant Release and Transfer Register (PRTR)**

not listed

**Directive 2000/60/EC establishing a framework for Community action in the field of water policy (WFD)**

not listed

##### National inventories

Substance is listed in the following national inventories:

- EINECS/ELINCS/NLP (Europe)
- REACH (Europe)

#### 15.2 Chemical Safety Assessment

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

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### SECTION 16: Other information

#### Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
ADN	Accord européen relatif au transport international des marchandises dangereuses par voies de navigation intérieures (European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways)
ADR	Accord européen relatif au transport international des marchandises dangereuses par route (European Agreement concerning the International Carriage of Dangerous Goods by Road)
BCF	BioConcentration Factor
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
CMR	Carcinogenic, Mutagenic or toxic for Reproduction
DMEL	Derived Minimal Effect Level
DNEL	Derived No-Effect Level
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
IMDG	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
MARPOL	International Convention for the Prevention of Pollution from Ships (abbr. of "Marine Pollutant")
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No-Effect Concentration
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RID	Règlement concernant le transport International ferroviaire des marchandises Dangereuses (Regulations concerning the International carriage of Dangerous goods by Rail)
S.I. No. 619 of 2001	Safety, Health and Welfare at Work (Chemical Agents) Regulations 2001
STEL	short-term exposure limit
TWA	time-weighted average
vPvB	very Persistent and very Bioaccumulative

#### Key literature references and sources for data

- Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU
- Regulation (EC) No. 1272/2008 (CLP, EU GHS)

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### List of relevant phrases (code and full text as stated in chapter 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

The above information describes exclusively the safety requirements of the product and is based on our present-day knowledge. The information is intended to give you advice about the safe handling of the product named in this safety data sheet, for storage, processing, transport and disposal. The information cannot be transferred to other products. In the case of mixing the product with other products or in the case of processing, the information on this safety data sheet is not necessarily valid for the new made-up material.