



SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 22.02.2013

Version 12.11

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

1.1 Product identifier

Catalogue No.	822292
Product name	4-Nitroaniline for synthesis
REACH Registration Number	A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

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

Identified uses	Chemical for synthesis For additional information on uses please refer to the Merck Chemicals portal (www.merck-chemicals.com).
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1.3 Details of the supplier of the safety data sheet

Company	Merck KGaA * 64271 Darmstadt * Germany * Phone:+49 6151 72-0
Responsible Department	EQ-RS * e-mail: prodsafe@merckgroup.com

1.4 Emergency telephone number **Please contact the regional company representation in your country.**

SECTION 2. Hazards identification

2.1 Classification of the substance or mixture

Classification (REGULATION (EC) No 1272/2008)

Acute toxicity, Category 3, Inhalation, H331
Acute toxicity, Category 3, Dermal, H311
Acute toxicity, Category 3, Oral, H301
Specific target organ toxicity - repeated exposure, Category 2, H373
Chronic aquatic toxicity, Category 3, H412

For the full text of the H-Statements mentioned in this Section, see Section 16.

Classification (67/548/EEC or 1999/45/EC)

T	Toxic	R23/24/25 R33 R52/53
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For the full text of the R-phrases mentioned in this Section, see Section 16.

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2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

Hazard pictograms



Signal word

Danger

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

Prevention

P273 Avoid release to the environment.
P280 Wear protective gloves/ protective clothing.

Response

P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
P302 + P352 IF ON SKIN: Wash with plenty of soap and water.
P309 + P310 IF exposed or if you feel unwell: Immediately call a POISON CENTER or doctor/physician.

Reduced labelling (≤ 125 ml)

Hazard pictograms



Signal word

Danger

Hazard statements

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

Precautionary statements

P280 Wear protective gloves/ protective clothing.
P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
P309 + P310 IF exposed or if you feel unwell: Immediately call a POISON CENTER or doctor/physician.

Index-No. 612-012-00-9

Labelling (67/548/EEC or 1999/45/EC)

Symbol(s)	T	Toxic
R-phrase(s)	23/24/25-33-52/53	Toxic by inhalation, in contact with skin and if swallowed. Danger of cumulative effects. Harmful to aquatic organisms, may cause long-term adverse effects in the aquatic environment.
S-phrase(s)	28-36/37-45-61	After contact with skin, wash immediately with plenty of soap

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and water. Wear suitable protective clothing and gloves. In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible). Avoid release to the environment. Refer to special instructions/ Safety data sheets.

EC-No. 202-810-1

EC Label

Reduced labelling (≤125 ml)

Symbol(s)  T

Toxic

R-phrases 23/24/25-52/53

Toxic by inhalation, in contact with skin and if swallowed. Harmful to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

S-phrases 36/37-45

Wear suitable protective clothing and gloves. In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).

2.3 Other hazards

None known.

SECTION 3. Composition/information on ingredients

3.1 Substance

Formula	H ₂ NC ₆ H ₄ NO ₂	C ₆ H ₆ N ₂ O ₂ (Hill)
CAS-No.	100-01-6	
Index-No.	612-012-00-9	
EC-No.	202-810-1	
Molar mass	138,13 g/mol	

Hazardous components (REGULATION (EC) No 1272/2008)

Chemical Name (Concentration)

CAS-No.	Registration number	Classification
4-Nitroaniline (<= 100 %)		
100-01-6	*)	Acute toxicity, Category 3, H331 Acute toxicity, Category 3, H311 Acute toxicity, Category 3, H301 Specific target organ toxicity - repeated exposure, Category 2, H373 Chronic aquatic toxicity, Category 3, H412

*) A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

For the full text of the H-Statements mentioned in this Section, see Section 16.

Hazardous components (1999/45/EC)

Chemical Name (Concentration)

CAS-No.	Classification
4-Nitroaniline (<= 100 %)	
100-01-6	T, Toxic; R23/24/25 R33 R52/53

For the full text of the R-phrases mentioned in this Section, see Section 16.

3.2 Mixture

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not applicable

SECTION 4. First aid measures

4.1 Description of first aid measures

General advice

First aider needs to protect himself.

After inhalation: fresh air. If breathing stops: immediately apply artificial respiration, if necessary oxygen. Immediately call in physician.

After skin contact: wash off with plenty of water. Remove contaminated clothing. Call a physician immediately.

After eye contact: rinse out with plenty of water with the eyelid held wide open. Call in ophthalmologist if necessary.

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

irritant effects, Cough, Shortness of breath, Drowsiness, Dizziness, Unconsciousness, agitation, Nausea, Vomiting, collapse, ataxia (impaired locomotor coordination)

4.3 Indication of any immediate medical attention and special treatment needed

Gastric lavage.

SECTION 5. Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Water, Carbon dioxide (CO₂), Foam, 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

Combustible.

Risk of dust explosion.

Vapours 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.

Fire may cause evolution of:

nitrous gases, nitrogen oxides

5.3 Advice for firefighters

Special protective equipment 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.

Further information

Suppress (knock down) gases/vapours/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

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SECTION 6. Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid inhalation of dusts in all circumstances. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders: Protective equipment see section 8.

6.2 Environmental precautions

Do not empty into 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. Dispose of properly. Clean up affected area. Avoid generation of dusts.

6.4 Reference to other sections

Indications about waste treatment 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.

Observe label precautions.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed. Dry. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorised persons.

Store at +15°C to +25°C.

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

8.2 Exposure controls

Engineering measures

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

See section 7.1.

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Individual protection measures

Protective clothing needs to be selected specifically for the workplace, depending on concentrations and quantities of the hazardous substances handled. The chemical resistance of the protective equipment should be enquired at the respective supplier.

Eye/face protection

Safety glasses

Hand protection

full contact:

Glove material:	Nitrile rubber
Glove thickness:	0,11 mm
Break through time:	> 480 min

splash contact:

Glove material:	Nitrile rubber
Glove thickness:	0,11 mm
Break through time:	> 480 min

The protective gloves to be used must comply with the specifications of EC Directive 89/686/EEC and the related standard EN374, for example KCL 741 Dermatril® L (full contact), KCL 741 Dermatril® L (splash contact).

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types.

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 EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Other protective equipment

protective clothing

Respiratory protection

required when dusts are generated.

Recommended Filter type: Filter A-(P2)

The entrepreneur 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.

Environmental exposure controls

Do not empty into drains.

SECTION 9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

Form	solid
Colour	yellow
Odour	odourless
Odour Threshold	not applicable
pH	at 0,5 g/l 20 °C neutral

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Melting point	148 °C
Boiling point/boiling range	> 331 °C at 1.013 hPa (decomposition)
Flash point	199 °C
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	No information available.
Upper explosion limit	No information available.
Vapour pressure	1,33 hPa at 142 °C
Relative vapour density	4,77
Relative density	1,44 g/cm ³ at 20 °C
Water solubility	0,5 g/l at 20 °C
Partition coefficient: n-octanol/water	log Pow: 1,39 OECD Test Guideline 107 Bioaccumulation is not expected.
Auto-ignition temperature	No information available.
Decomposition temperature	> 310 °C
Viscosity, dynamic	No information available.
Explosive properties	No information available.
Oxidizing properties	No information available.

9.2 Other data

Ignition temperature	500 °C
Bulk density	ca.630 kg/m ³

SECTION 10. Stability and reactivity

10.1 Reactivity

Risk of dust explosion.
Forms explosive mixtures with air on intense heating.

10.2 Chemical stability

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heat-sensitive
sensitive to moisture

10.3 Possibility of hazardous reactions

Risk of ignition or formation of inflammable gases or vapours with:

Organic Substances, magnesium, Nitric acid

Exothermic reaction with:

sulphuric acid

Risk of explosion with:

Sodium hydroxide, organic nitro compounds, Ether

Violent reactions possible with:

strong reducing agents, Bases, Acid chlorides, Acid anhydrides

Caution! In contact with nitrites, nitrates, nitrous acid possible liberation of nitosamines!

10.4 Conditions to avoid

Strong heating.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

10.5 Incompatible materials

rubber, various plastics

10.6 Hazardous decomposition products

in the event of fire: See section 5.

SECTION 11. Toxicological information

11.1 Information on toxicological effects

Acute oral toxicity

LD50 rat: 750 mg/kg (RTECS) (Regulation (EC) No 1272/2008, Annex VI)

absorption

Symptoms: Nausea, Vomiting, Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.

Acute inhalation toxicity

absorption

Symptoms: mucosal irritations, Cough, Shortness of breath

Acute dermal toxicity

LD50 rabbit: > 2.500 mg/kg (External MSDS) (Regulation (EC) No 1272/2008, Annex VI)

absorption

Skin irritation

rabbit

Result: No irritation

OECD Test Guideline 404

Eye irritation

rabbit

Result: No eye irritation

OECD Test Guideline 405

Sensitisation

This information is not available.

Germ cell mutagenicity

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Genotoxicity in vitro

Mutagenicity (mammal cell test):
Result: positive
(National Toxicology Program)

Ames test
Salmonella typhimurium
Result: positive
(National Toxicology Program)

Carcinogenicity

This information is not available.

Reproductive toxicity

This information is not available.

Teratogenicity

This information is not available.

Specific target organ toxicity - single exposure

This information is not available.

Specific target organ toxicity - repeated exposure

May cause damage to organs through prolonged or repeated exposure.

Aspiration hazard

This information is not available.

11.2 Further information

Systemic effects:

Dizziness, ataxia (impaired locomotor coordination), Drowsiness, agitation, collapse, Unconsciousness, Changes in the blood count, Risk of methaemoglobin formation with headache, cardiac dysrhythmia, drop in blood pressure, dyspnoea and spasms, principal symptom: cyanosis (blue discolouration of the blood).

Damage to:

Liver, Kidney, Central nervous system

Effect potentiated by: ethanol

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

12.1 Toxicity

Toxicity to fish

LC50 Danio rerio (zebra fish): 87,6 mg/l; 96 h (IUCLID)

Toxicity to daphnia and other aquatic invertebrates

EC50 Daphnia magna (Water flea): 17 mg/l; 48 h (ECOTOX Database)

12.2 Persistence and degradability

Biodegradability

> 95 %; 14 d

OECD Test Guideline 302B

Readily eliminated from water

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 1,39

OECD Test Guideline 107

Bioaccumulation is not expected.

12.4 Mobility in soil

No information available.

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12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted.

12.6 Other adverse effects

Additional ecological information

Discharge into the environment must be avoided.

SECTION 13. Disposal considerations

Waste treatment methods

See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14. Transport information

Land transport (ADR/RID)

14.1 UN number	UN 1661
14.2 Proper shipping name	NITROANILINES
14.3 Class	6.1
14.4 Packing group	II
14.5 Environmentally hazardous	--
14.6 Special precautions for user	yes
Tunnel restriction code	D/E

Inland waterway transport (ADN)

Not relevant

Air transport (IATA)

14.1 UN number	UN 1661
14.2 Proper shipping name	NITROANILINES
14.3 Class	6.1
14.4 Packing group	II
14.5 Environmentally hazardous	--
14.6 Special precautions for user	no

Sea transport (IMDG)

14.1 UN number	UN 1661
14.2 Proper shipping name	NITROANILINES
14.3 Class	6.1
14.4 Packing group	II
14.5 Environmentally hazardous	--
14.6 Special precautions for user	yes
EmS	F-A S-A

14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not relevant

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SECTION 15. Regulatory information

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

EU regulations

Major Accident Hazard 96/82/EC
Legislation Toxic
2
Quantity 1: 50 t
Quantity 2: 200 t

Occupational restrictions Take note of Dir 94/33/EC on the protection of young people at work. Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.

National legislation

Storage class 6.1A

15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out.

SECTION 16. Other information

Full text of H-Statements referred to under sections 2 and 3.

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.

Full text of R-phrases referred to under sections 2 and 3

R23/24/25 Toxic by inhalation, in contact with skin and if swallowed.
R33 Danger of cumulative effects.
R52/53 Harmful to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

Training advice

Provide adequate information, instruction and training for operators.

Key or legend to abbreviations and acronyms used in the safety data sheet

Used abbreviations and acronyms can be looked up at www.wikipedia.org.

Regional representation

This information is given on the authorised Safety Data Sheet for your country.

The information contained herein is based on the present state of our knowledge. It characterises the product with regard to the appropriate safety precautions. It does not represent a guarantee of any properties of the product.