

Safety data sheet

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



p-Nitrotoluene ≥98 %, for synthesis

article number: **0881**
Version: **2.0 en**
Replaces version of: 06.09.2018
Version: (1)

date of compilation: 06.09.2018
Revision: 29.04.2019

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

1.1 Product identifier

| | |
|---------------------------------|--|
| Identification of the substance | p-Nitrotoluene |
| Article number | 0881 |
| 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 No | 609-006-00-3 |
| EC number | 202-808-0 |
| CAS number | 99-99-0 |

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

Identified uses: laboratory chemical
laboratory and analytical use

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

Website: www.carlroth.de

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

e-mail (competent person) : 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 |

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| Classification acc. to GHS | | | |
|----------------------------|---|---------------------------|------------------|
| Section | Hazard class | Hazard class and category | Hazard statement |
| 4.1C | hazardous to the aquatic environment - chronic hazard | (Aquatic Chronic 2) | H411 |

2.2 Label elements

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

Signal word **Danger**

Pictograms

GHS06, GHS08,
GHS09



Hazard statements

H301+H311+H331 Toxic if swallowed, in contact with skin or if inhaled
H373 May cause damage to organs (liver, testes) through prolonged or repeated exposure
H411 Toxic to aquatic life with long lasting effects

Precautionary statements

Precautionary statements - prevention

P270 Do not eat, drink or smoke when using this product.
P273 Avoid release to the environment.
P280 Wear protective gloves/eye protection.

Precautionary statements - response

P302+P352 IF ON SKIN: Wash with plenty of water.
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P310 Immediately call a POISON CENTER/doctor.

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.
P270 Do not eat, drink or smoke when using this product.
P280 Wear protective gloves/eye 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.

2.3 Other hazards

There is no additional information.

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SECTION 3: Composition/information on ingredients

3.1 Substances

| | |
|-------------------|---|
| Name of substance | p-Nitrotoluene |
| Index No | 609-006-00-3 |
| EC number | 202-808-0 |
| CAS number | 99-99-0 |
| Molecular formula | C ₇ H ₇ NO ₂ |
| Molar mass | 137,1 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. In case of extensive skin contact serious poisoning possible. Call a physician in any case.

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

Cardiac arrhythmias, Headache, Spasms, Dyspnoea, Methaemoglobinaemia, Blood pressure drop, Cyanosis (blue coloured blood)

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 fire-fighting measures to the fire surroundings

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water spray, foam, dry extinguishing powder, carbon dioxide (CO₂)

Unsuitable extinguishing media

water jet

5.2 Special hazards arising from the substance or mixture

Combustible. Vapours may form explosive mixtures with air. Vapours are heavier than air.

Hazardous combustion products

In case of fire may be liberated: nitrogen oxides (NO_x), carbon monoxide (CO), carbon dioxide (CO₂)

5.3 Advice for firefighters

Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus. Wear full chemical protective clothing. Do not allow firefighting water to enter drains or water courses.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures



For non-emergency personnel

Avoid dust formation. Do not breathe dust. 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. Provide adequate ventilation.

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

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.

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

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

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

Keep container tightly closed. Store in a dry place.

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Incompatible substances or mixtures

Observe hints for combined storage.

Consideration of other advice

Store locked up.

• Ventilation requirements

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)

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 (crystalline) |
| Colour | yellow |
| Odour | characteristic |
| Odour threshold | No data available |

Other physical and chemical parameters

| | |
|---|--|
| pH (value) | This information is not available. |
| Melting point/freezing point | 52 – 54 °C |
| Initial boiling point and boiling range | 238 – 240 °C |
| Flash point | 103 °C at 1.013 hPa |
| Evaporation rate | no data available |
| Flammability (solid, gas) | These information are not available |
| <u>Explosive limits</u> | |
| • lower explosion limit (LEL) | 1,6 vol% |
| • upper explosion limit (UEL) | this information is not available |
| Explosion limits of dust clouds | these information are not available |
| Vapour pressure | <0,2 hPa at 20 °C |
| Density | 1,1 – 1,2 g/cm ³ at 20 °C |
| Vapour density | This information is not available. |
| Relative density | Information on this property is not available. |
| <u>Solubility(ies)</u> | |
| Water solubility | <0,5 g/l at 20 °C |
| <u>Partition coefficient</u> | |
| n-octanol/water (log KOW) | 2,37 (25 °C) (ECHA) |
| Auto-ignition temperature | >450 °C |
| Decomposition temperature | no data available |
| Viscosity | not relevant (solid matter) |

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| | |
|----------------------|--------------------------------------|
| Explosive properties | Shall not be classified as explosive |
| Oxidising properties | none |

9.2 Other information

There is no additional information.

SECTION 10: Stability and reactivity

10.1 Reactivity

If heated: Vapours can form explosive mixtures with air, Dust explosibility

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 alkali, Strong oxidiser, Ammonia (NH₃), Strong acid, Reducing agents, Sulphur trioxide,
=> Explosive properties

10.4 Conditions to avoid

Keep away from heat.

10.5 Incompatible materials

plastic and rubber

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 | 1.960 mg/kg | rat | TOXNET |
| dermal | LD50 | >16.000 mg/kg | rabbit | TOXNET |

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

• 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 (liver, testes) through prolonged or repeated exposure.

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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

causes slight to moderate irritation

• If inhaled

irritant effects, headache

• If on skin

causes slight to moderate irritation, risk of absorption via the skin

Other information

Other adverse effects: Cardiac arrhythmias. Dyspnoea. Blood pressure drop. Spasms. Methaemoglobinemia. Cyanosis (blue coloured blood).

SECTION 12: Ecological information

12.1 Toxicity

Toxic to aquatic life with long lasting effects.

Aquatic toxicity (acute)

| Endpoint | Value | Species | Source | Exposure time |
|----------|----------|-----------------------|--------|---------------|
| EC50 | 4,2 mg/l | daphnia magna | ECHA | 48 h |
| ErC50 | 22 mg/l | Chlorella pyrenoidosa | ECHA | 96 h |

Aquatic toxicity (chronic)

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

| Endpoint | Value | Species | Source | Exposure time |
|----------|--------|----------------|--------|---------------|
| EC50 | 5 mg/l | microorganisms | ECHA | 15 min |

12.2 Process of degradability

Theoretical Oxygen Demand with nitrification: 2,042 mg/mg

Theoretical Oxygen Demand: 1,633 mg/mg

Theoretical Carbon Dioxide: 2,246 mg/mg

| Process | Degradation rate | Time |
|------------------|------------------|------|
| DOC removal | 94 % | 15 d |
| oxygen depletion | 0,8 % | 14 d |

12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW) 2,37 (25 °C)

BCF 39,26

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12.4 Mobility in soil

Henry's law constant $2,38 \text{ Pa m}^3/\text{mol}$ at 25 °C

12.5 Results of PBT and vPvB assessment

Data are not available.

12.6 Other adverse effects

Data are not available.

Endocrine disrupting potential

| Name of substance | CAS No | Combined category | Human health category | Wildlife category |
|-------------------|---------|-------------------|-----------------------|-------------------|
| p-Nitrotoluene | 99-99-0 | CAT1 | CAT1 | CAT3 |

Legend

CAT1 Category 1 - evidence of endocrine disruption in at least one species using intact animals
CAT3 Category 3 - no evidence of endocrine disruption or no data 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.

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.

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SECTION 14: Transport information

| | | |
|-------------|---|---|
| 14.1 | UN number | 3446 |
| 14.2 | UN proper shipping name Hazardous ingredients | NITROTOLUENES, SOLID p-Nitrotoluene |
| 14.3 | Transport hazard class(es) |  |
| | Class | 6.1 (toxic substances) |
| 14.4 | Packing group | II (substance presenting medium danger) |
| 14.5 | Environmental hazards | hazardous to the aquatic environment |
| 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 | 3446 |
| | Proper shipping name | NITROTOLUENES, SOLID |
| | Particulars in the transport document | UN3446, NITROTOLUENES, SOLID, 6.1, II, (D/E), environmentally hazardous |
| | Class | 6.1 |
| | Classification code | T2 |
| | Packing group | II |
| | Danger label(s) | 6.1 + "fish and tree" |
| |   | |
| | Environmental hazards | yes (hazardous to the aquatic environment) |
| | Special provisions (SP) | 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 | 3446 |
| | Proper shipping name | NITROTOLUENES, SOLID |



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| | |
|---|---|
| Particulars in the shipper's declaration | UN3446, NITROTOLUENES, SOLID, 6.1, II, MARINE POLLUTANT |
| Class | 6.1 |
| Marine pollutant | yes (P) (hazardous to the aquatic environment) |
| Packing group | II |
| Danger label(s) | 6.1 + "fish and tree" |
|  | |
| Special provisions (SP) | - |
| Excepted quantities (EQ) | E4 |
| Limited quantities (LQ) | 500 g |
| EmS | F-A, S-A |
| Stowage category | A |
| • International Civil Aviation Organization (ICAO-IATA/DGR) | |
| UN number | 3446 |
| Proper shipping name | Nitrotoluenes, solid |
| Particulars in the shipper's declaration | UN3446, Nitrotoluenes, solid, 6.1, II |
| Class | 6.1 |
| Environmental hazards | yes (hazardous to the aquatic environment) |
| Packing group | II |
| Danger label(s) | 6.1 |
|  | |
| Excepted quantities (EQ) | E4 |
| Limited quantities (LQ) | 1 kg |

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**

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not listed

• Restrictions according to REACH, Title VIII

None.

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

not listed

• Directive 75/324/EEC relating to aerosol dispensers

Filling batch

Deco-Paint Directive (2004/42/EC)

| | |
|-------------|--------------------|
| VOC content | 100 % 1.200 g/l |
|-------------|--------------------|

Directive on industrial emissions (VOCs, 2010/75/EU)

| | |
|-------------|-----------|
| VOC content | 100 % |
| VOC content | 1.200 g/l |

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

Regulation 98/2013/EU on the marketing and use of explosives precursors

not listed

Regulation 111/2005/EC laying down rules for the monitoring of trade between the Community and third countries in drug precursors

not listed

National inventories

Substance is listed in the following national inventories:

| Country | National inventories | Status |
|---------|----------------------|---------------------|
| AU | AICS | 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 |
| NZ | NZIoC | substance is listed |
| PH | PICCS | substance is listed |

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| Country | National inventories | Status |
|---------|----------------------|---------------------|
| TW | TCSI | substance is listed |
| US | TSCA | substance is listed |

Legend

| | |
|------------|---|
| AICS | Australian Inventory of Chemical Substances |
| 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 |
| KECI | Korea Existing Chemicals Inventory |
| NZIoC | New Zealand Inventory of Chemicals |
| PICCS | Philippine Inventory of Chemicals and Chemical Substances |
| 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.

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 |
| DGR | Dangerous Goods Regulations (see IATA/DGR) |
| 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 |
| 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 |
| REACH | Registration, Evaluation, Authorisation and Restriction of Chemicals |

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| Abbr. | Descriptions of used abbreviations |
|-------|---|
| RID | Règlement concernant le transport International ferroviaire des marchandises Dangereuses (Regulations concerning the International carriage of Dangerous goods by Rail) |
| SVHC | Substance of Very High Concern |
| VOC | Volatile Organic Compounds |
| 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)
- Dangerous Goods Regulations (DGR) for the air transport (IATA)
- International Maritime Dangerous Goods Code (IMDG)

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 (liver, testes) through prolonged or repeated exposure |
| H411 | toxic 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.