SAFETY DATA SHEET

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

1.1 Product identifiers

Product name: 4-Nitrotoluene

Product Number: N27322
Brand: Aldrich
Index-No.: 609-006-00-3
CAS-No.: 99-99-0

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

Identified uses: Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company: Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone: +1 314 771-5765
Fax: +1 800 325-5052

1.4 Emergency telephone

Emergency Phone #: 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Acute toxicity, Oral (Category 3), H301
Acute toxicity, Inhalation (Category 3), H331
Acute toxicity, Dermal (Category 3), H311
Specific target organ toxicity - repeated exposure (Category 2), H373
Short-term (acute) aquatic hazard (Category 2), H401
Long-term (chronic) aquatic hazard (Category 2), H411

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

2.2 GHS Label elements, including precautionary statements

Pictogram
Signal word: Danger

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

Precautionary statement(s):
- P260: Do not breathe dust/ fume/ gas/ mist/ vapors/ spray.
- P264: Wash skin thoroughly after handling.
- P270: Do not eat, drink or smoke when using this product.
- P271: Use only outdoors or in a well-ventilated area.
- P273: Avoid release to the environment.
- P280: Wear protective gloves/ protective clothing.
- P302 + P352 + P312: IF ON SKIN: Wash with plenty of water. Call a POISON CENTER/ doctor if you feel unwell.
- P304 + P340 + P311: IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor.
- P314: Get medical advice/ attention if you feel unwell.
- P362: Take off contaminated clothing and wash before reuse.
- P391: Collect spillage.
- P403 + P233: Store in a well-ventilated place. Keep container tightly closed.
- P405: Store locked up.
- P501: Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

SECTION 3: Composition/information on ingredients

3.1 Substances

<table>
<thead>
<tr>
<th>Synonyms</th>
<th>1-Methyl-4-nitrobenzene</th>
</tr>
</thead>
<tbody>
<tr>
<td>Formula</td>
<td>C₇H₇NO₂</td>
</tr>
<tr>
<td>Molecular weight</td>
<td>137.14 g/mol</td>
</tr>
<tr>
<td>CAS-No.</td>
<td>99-99-0</td>
</tr>
<tr>
<td>EC-No.</td>
<td>202-808-0</td>
</tr>
<tr>
<td>Index-No.</td>
<td>609-006-00-3</td>
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</table>

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
</tr>
</thead>
<tbody>
<tr>
<td>4-nitrotoluene</td>
<td>Acute Tox. 3; STOT RE 2; Aquatic Acute 2; Aquatic Chronic 2; H301, H331, H311, H373, H401, H411</td>
</tr>
</tbody>
</table>

For the full text of the H-Statements mentioned in this Section, see Section 16.
SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice
Consult a physician. Show this material safety data sheet to the doctor in attendance. Move out of dangerous area.

If inhaled
If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact
Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

In case of eye contact
Flush eyes with water as a precaution.

If swallowed
Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed
The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed
No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media
Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture
Carbon oxides
Nitrogen oxides (NOx)

5.3 Advice for firefighters
Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information
No data available

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures
Wear respiratory protection. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust. For personal protection see section 8.

6.2 Environmental precautions
Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.
6.3 Methods and materials for containment and cleaning up
Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

6.4 Reference to other sections
For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling
Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Advice on safe handling
Further processing of solid materials may result in the formation of combustible dusts. The potential for combustible dust formation should be taken into consideration before additional processing occurs.

Advice on protection against fire and explosion
Provide appropriate exhaust ventilation at places where dust is formed.

Hygiene measures
Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions
Keep container tightly closed in a dry and well-ventilated place.

Storage class
Storage class (TRGS 510): 6.1B: Non-combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials

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

Ingredients with workplace control parameters

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>4-nitrotoluene</td>
<td>99-99-0</td>
<td>TWA</td>
<td>2 ppm 11 mg/m3</td>
<td>USA. NIOSH Recommended Exposure Limits</td>
</tr>
</tbody>
</table>

Remarks: Potential for dermal absorption

<table>
<thead>
<tr>
<th></th>
<th>TWA</th>
<th>5 ppm 30 mg/m3</th>
<th>USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants</th>
</tr>
</thead>
</table>

Skin designation

<table>
<thead>
<tr>
<th></th>
<th>TWA</th>
<th>2 ppm</th>
<th>USA. ACGIH Threshold Limit Values (TLV)</th>
</tr>
</thead>
</table>

Danger of cutaneous absorption
<table>
<thead>
<tr>
<th>PEL</th>
<th>2 ppm 11 mg/m³</th>
<th>California permissible exposure limits for chemical contaminants (Title 8, Article 107)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Skin</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### 8.2 Exposure controls

**Appropriate engineering controls**
Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

**Personal protective equipment**

**Eye/face protection**
Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

**Skin protection**
Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Full contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested:Dermatril® (KCL 740 / Aldrich Z677272, Size M)

Splash contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested:Dermatril® (KCL 740 / Aldrich Z677272, Size M)

**Body Protection**
Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

**Respiratory protection**
Where risk assessment shows air-purifying respirators are appropriate use a full-face particle respirator type N99 (US) or type P2 (EN 143) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).
Control of environmental exposure
Prevent further leakage or spillage if safe to do so. Do not let product enter drains.
Discharge into the environment must be avoided.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Appearance
   Form: crystalline
   Color: light yellow

b) Odor
   No data available

c) Odor Threshold
   No data available

d) pH
   No data available

e) Melting point/freezing point
   Melting point/range: 52 - 54 °C (126 - 129 °F) - lit.

f) Initial boiling point and boiling range
   238 °C 460 °F - lit.

g) Flash point
   106.00 °C (222.80 °F) - closed cup

h) Evaporation rate
   No data available

i) Flammability (solid, gas)
   The product is not flammable. - Flammability (solids)

j) Upper/lower flammability or explosive limits
   Lower explosion limit: 1.6 %(V)

k) Vapor pressure
   0.13 hPa at 20 °C (68 °F)

l) Vapor density
   5.49

m) Density
   1.392 g/cm3 at 25 °C (77 °F) - lit.
   Relative density
   No data available

n) Water solubility
   0.345 g/l at 20 °C (68 °F)

o) Partition coefficient: n-octanol/water
   log Pow: 2.37 at 25 °C (77 °F)

p) Autoignition temperature
   450 °C (842 °F)

q) Decomposition temperature
   No data available

r) Viscosity
   No data available

s) Explosive properties
   No data available

t) Oxidizing properties
   No data available

9.2 Other safety information

Relative vapor density
5.49
SECTION 10: Stability and reactivity

10.1 Reactivity
No data available

10.2 Chemical stability
Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions
No data available

10.4 Conditions to avoid
No data available

10.5 Incompatible materials
Oxidizing agents, Reducing agents, Strong bases

10.6 Hazardous decomposition products
In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity
LD50 Oral - Rat - male and female - > 2,250 mg/kg
(OECD Test Guideline 401)
Acute toxicity estimate Inhalation - 4 h - 0.51 mg/l
(Expert judgment)
LD50 Dermal - Rat - > 16,000 mg/kg
Remarks: Lungs, Thorax, or Respiration: Other changes.
Liver: Fatty liver degeneration.
Nutritional and Gross Metabolic: Weight loss or decreased weight gain.
No data available

Skin corrosion/irritation
Skin - Rabbit
Result: No skin irritation - 4 h
(OECD Test Guideline 404)

Serious eye damage/eye irritation
Eyes - Rabbit
Result: No eye irritation - 24 h
(OECD Test Guideline 405)

Respiratory or skin sensitization
Buehler Test - Guinea pig
Result: Does not cause skin sensitization.
(OECD Test Guideline 406)

Germ cell mutagenicity
Test Type: Ames test
Test system: S. typhimurium
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 471
Result: negative
Test Type: In vivo micronucleus test  
Species: Rat

Application Route: Intraperitoneal  
Method: Mutagenicity (micronucleus test)  
Result: negative

**Carcinogenicity**

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA’s list of regulated carcinogens.

**Reproductive toxicity**

No data available

**Specific target organ toxicity - single exposure**

No data available

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**11.2 Additional Information**

RTECS: XT3325000  
Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea, Vomiting, burning sensation, Absorption into the body leads to the formation of methemoglobin which in sufficient concentration causes cyanosis. Onset may be delayed 2 to 4 hours or longer. To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

**SECTION 12: Ecological information**

**12.1 Toxicity**

Toxicity to fish  
LC50 - Pimephales promelas (fathead minnow) - 49.7 mg/l - 96.0 h

Toxicity to daphnia and other aquatic invertebrates  
Immobilization EC50 - Daphnia magna (Water flea) - ca. 4.2 mg/l - 48 h (ISO 6341)

Toxicity to algae  
static test EC50 - Chlorella pyrenoidosa - 22 mg/l - 96 h (OECD Test Guideline 201)

**12.2 Persistence and degradability**

Biodegradability  
aerobic - Exposure time 14 d  
Result: 0.8 % - According to the results of tests of biodegradability this product is not readily biodegradable.
12.3 Bioaccumulative potential
No data available

12.4 Mobility in soil
No data available

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
Toxic to aquatic life with long lasting effects.
An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.
No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product
Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

Contaminated packaging
Dispose of as unused product.

SECTION 14: Transport information

DOT (US)
UN number: 3446  Class: 6.1  Packing group: II
Proper shipping name: Nitrotoluenes, solid
Reportable Quantity (RQ): 1000 lbs
Poison Inhalation Hazard: No

IMDG
UN number: 3446  Class: 6.1  Packing group: II
Proper shipping name: NITROTOLUENES, SOLID
EMS-No: F-A, S-A

IATA
UN number: 3446  Class: 6.1  Packing group: II
Proper shipping name: Nitrotoluenes, solid

SECTION 15: Regulatory information

SARA 302 Components
No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components
This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

**SARA 311/312 Hazards**
Acute Health Hazard, Chronic Health Hazard

**Massachusetts Right To Know Components**
No components are subject to the Massachusetts Right to Know Act.

**Pennsylvania Right To Know Components**

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>4-nitrotoluene</td>
<td>99-99-0</td>
<td>1994-04-01</td>
</tr>
</tbody>
</table>

**SECTION 16: Other information**

**Further information**
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