

1. PRODUCT AND COMPANY IDENTIFICATION

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
3050 Spruce Street
SAINT LOUIS MO 63103
USA

Telephone : +1 800-325-5832

Fax : +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

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

Acute aquatic toxicity (Category 2), H401

Chronic aquatic toxicity (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
H373
H411

Toxic if swallowed, in contact with skin or if inhaled.
May cause damage to organs through prolonged or repeated exposure.
Toxic to aquatic life with long lasting effects.

Precautionary statement(s)

P260
P264
P270
P271

Do not breathe dust/ fume/ gas/ mist/ vapours/ spray.
Wash skin thoroughly after handling.
Do not eat, drink or smoke when using this product.
Use only outdoors or in a well-ventilated area.

P273	Avoid release to the environment.
P280	Wear protective gloves/ protective clothing.
P301 + P310	IF SWALLOWED: Immediately call a POISON CENTER/doctor.
P302 + P352	IF ON SKIN: Wash with plenty of soap and water.
P304 + P340	IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
P314	Get medical advice/ attention if you feel unwell.
P322	Specific measures (see supplemental first aid instructions on this label).
P330	Rinse mouth.
P361	Remove/Take off immediately all contaminated clothing.
P363	Wash contaminated clothing 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

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms	:	1-Methyl-4-nitrobenzene
Formula	:	C ₇ H ₇ NO ₂
Molecular weight	:	137.14 g/mol
CAS-No.	:	99-99-0
EC-No.	:	202-808-0
Index-No.	:	609-006-00-3

Hazardous components

Component	Classification	Concentration
4-Nitrotoluene	Acute Tox. 3; STOT RE 2; Aquatic Acute 2; Aquatic Chronic 2; H301 + H311 + H331, H373, H411	90 - 100 %

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

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice

Consult a physician. Show this 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

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

No data available

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

No data available

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Wear respiratory protection. Avoid dust formation. Avoid breathing vapours, 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.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid formation of dust and aerosols. 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. Provide appropriate exhaust ventilation at places where dust is formed. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

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

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
4-Nitrotoluene	99-99-0	TWA	2.000000 ppm 11.000000 mg/m3	USA. NIOSH Recommended Exposure Limits
	Remarks	Potential for dermal absorption		
		TWA	5.000000 ppm 30.000000 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		Skin designation		

		The value in mg/m3 is approximate.		
		TWA	5.000000 ppm 30.000000 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		Skin designation The value in mg/m3 is approximate.		
		TWA	2.000000 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Methemoglobinemia Substances for which there is a Biological Exposure Index or Indices (see BEI® section), see BEI® for Methemoglobin Inducers Danger of cutaneous absorption		
		TWA	5 ppm 30 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		Skin designation The value in mg/m3 is approximate.		
		PEL	2 ppm 11 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		
		TWA	2 ppm 11 mg/m3	USA. NIOSH Recommended Exposure Limits
		Potential for dermal absorption		
		TWA	2 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Methemoglobinemia Substances for which there is a Biological Exposure Index or Indices (see BEI® section), see BEI® for Methemoglobin Inducers Danger of cutaneous absorption		

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: Dermatrill® (KCL 740 / Aldrich Z677272, Size M)

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: Dermatrill® (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

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.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a) Appearance	Form: crystalline Colour: light yellow
b) Odour	No data available
c) Odour 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) Vapour pressure	0.13 hPa (0.10 mmHg) at 20 °C (68 °F)
l) Vapour density	5.49
m) Relative density	1.392 g/cm ³ at 25 °C (77 °F)
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) Auto-ignition 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 vapour density	5.49
-------------------------	------

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

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NO_x)

Other decomposition products - No data available

In the event of fire: see section 5

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)

LCLO Inhalation - Rat - 1 h - 4 ppm

LC50 Inhalation - Rat - 975 mg/m³

Remarks: Brain and Coverings:Recordings from specific areas of CNS. Liver:Fatty liver degeneration.

Blood:Methemoglobinemia-Carboxyhemoglobin.

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 sensitisation

Buehler Test - Guinea pig

Result: Does not cause skin sensitisation.

(OECD Test Guideline 406)

Germ cell mutagenicity

Ames test

S. typhimurium

Result: negative

Mutagenicity (micronucleus test)

Rat - male

Result: negative

Carcinogenicity

IARC: No component 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 component 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

Reproductive toxicity - Rat - Oral

Paternal Effects: Spermatogenesis (including genetic material, sperm morphology, motility, and count). Paternal Effects: Testes, epididymis, sperm duct.

Reproductive toxicity - Rat - Intraperitoneal

Maternal Effects: Uterus, cervix, vagina.

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

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.

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

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 (aglae) - 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. (OECD Test Guideline 301C)
------------------	--

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.

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.

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 EMS-No: F-A, S-A
Proper shipping name: NITROTOLUENES, SOLID

IATA

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

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

	CAS-No.	Revision Date
4-Nitrotoluene	99-99-0	1994-04-01

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
4-Nitrotoluene	99-99-0	1994-04-01

New Jersey Right To Know Components

	CAS-No.	Revision Date
4-Nitrotoluene	99-99-0	1994-04-01

California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

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

Acute Tox.	Acute toxicity
Aquatic Acute	Acute aquatic toxicity
Aquatic Chronic	Chronic aquatic toxicity
H301	Toxic if swallowed.
H301 + H311 + H331	Toxic if swallowed, in contact with skin or if inhaled.
H311	Toxic in contact with skin.
H331	Toxic if inhaled.
H373	May cause damage to organs through prolonged or repeated exposure.

HMIS Rating

Health hazard: 2
Chronic Health Hazard: *

Flammability: 1
Physical Hazard 0

NFPA Rating

Health hazard: 2
Fire Hazard: 1
Reactivity Hazard: 0

Further information

Copyright 2016 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only. The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Preparation Information

Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

Version: 4.7

Revision Date: 01/08/2018

Print Date: 11/10/2018