SAFETY DATA SHEET

1. PRODUCT

1.1 Product identifiers

Name: 4-Nitrotoluene 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

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 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/ vapours/ 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. 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

No data available

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms: 1-Methyl-4-nitrobenzene

Formula: $C_7H_7NO_2$ Molecular weight: 137.14 g/mol CAS-No.: 99-99-0 EC-No.: 202-808-0

Hazardous components

Component	Classification	Concentration
4-Nitrotoluene	6	
	Acute Tox. 3; STOT RE 2; Aquatic Acute 2; Aquatic Chronic 2; H301 + H311 + H331, H373, H411	<= 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

4.2 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.

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 designatio	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 designatio	n The value in m	g/m3 is approximate.		
TWA 2.000000 ppm USA. ACGIH Threshold Lin		USA. ACGIH Threshold Limit Values (TLV)				
A30010		Indices (see BE	lethemoglobinemia Substances for which there is a Biological Exposure Index or Indices (see BEI® section), see BEI® for Methemoglobin Inducers Danger of utaneous absorption			
0,		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				

# 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) 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 environmen tal 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

Appearance	Form: crystalline Colour: light yellow
Odour	No data available
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	Melting point/range: 51 - 53 °C (124 - 127 °F)
Initial boiling point and boiling range	238 °C (460 °F)
Flash point	106.00 °C (222.80 °F) - closed cup
Evaporation rate	No data available
Flammability (solid, gas)	The product is not flammable Flammability (solids)
Upper/lower flammability or explosive limits	Lower explosion limit: 1.6 %(V)
Vapour pressure	0.13 hPa (0.10 mmHg) at 20 °C (68 °F)
Vapour density	5.49
Relative density	1.392 g/mL at 25 °C (77 °F)
Water solubility	0.345 g/l at 20 °C (68 °F)
Partition coefficient: n-octanol/water	log Pow: 2.37 at 25 °C (77 °F)
Auto-ignition temperature	450 °C (842 °F)
Decomposition temperature	No data available
Viscosity	No data available
Explosive properties	No data available
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 (NOx)

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

Eves - 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 identified as a carcinogen or potential carcinogen by OSHA.

# 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
	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)
Toxicity to bacteria	No data available

### 12.2 Persistence and degradability

 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**

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

# Pennsylvania Right To Know Components

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

# **New Jersey Right To Know Components**

Component	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