

## SAFETY DATA SHEET

Version 8.7  
Revision Date 08/06/2024  
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**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : 3-Nitrotoluene

Product Number : N27314  
Brand : Aldrich  
CAS-No. : 99-08-1

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

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

**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 4), H302  
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

Warning

Hazard Statements

H302

Harmful if swallowed.

H373

May cause damage to organs through prolonged or repeated exposure.

H411

Toxic to aquatic life with long lasting effects.

Precautionary Statements

P260

Do not breathe mist or vapors.

P264

Wash skin thoroughly after handling.

P270

Do not eat, drink or smoke when using this product.

P273

Avoid release to the environment.

P301 + P312 + P330

IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.

P314

Get medical advice/ attention if you feel unwell.

P391

Collect spillage.

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

Synonyms : 1-Methyl-3-nitrobenzene

Formula :  $C_7H_7NO_2$

Molecular weight : 137.14 g/mol

CAS-No. : 99-08-1

EC-No. : 202-728-6

Component	Classification	Concentration
<b>3-nitrotoluene</b>		
	Acute Tox. 4; STOT RE 2; Aquatic Acute 2; Aquatic Chronic 2; H302, H373, H401, H411	<= 100 %

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

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## **SECTION 4: First aid measures**

### **4.1 Description of first-aid measures**

No data available

### **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

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## **SECTION 5: Firefighting measures**

### **5.1 Extinguishing media**

No data available

### **5.2 Special hazards arising from the substance or mixture**

Carbon oxides

Nitrogen oxides (NO<sub>x</sub>)

Combustible.

### **5.3 Advice for firefighters**

No data available

### **5.4 Further information**

No data available

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## **SECTION 6: Accidental release measures**

### **6.1 Personal precautions, protective equipment and emergency procedures**

For personal protection see section 8.

### **6.2 Environmental precautions**

No data available

### **6.3 Methods and materials for containment and cleaning up**

No data available

### **6.4 Reference to other sections**

For disposal see section 13.

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## **SECTION 7: Handling and storage**

### **7.1 Precautions for safe handling**

For precautions see section 2.2.

### **7.2 Conditions for safe storage, including any incompatibilities**

No data available

### **7.3 Specific end use(s)**

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### Ingredients with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
3-nitrotoluene	99-08-1	TWA	2 ppm 11 mg/m <sup>3</sup>	USA. NIOSH Recommended Exposure Limits
	Remarks	Potential for dermal absorption		
		TWA	5 ppm 30 mg/m <sup>3</sup>	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		Skin designation		
		TWA	2 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Danger of cutaneous absorption		
		PEL	2 ppm 11 mg/m <sup>3</sup>	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		

#### Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
3-nitrotoluene	99-08-1	Methemoglobin	5% Hb	In blood	ACGIH - Biological Exposure Indices (BEI)
	Remarks	During or at the end of the shift			

### 8.2 Exposure controls

#### Personal protective equipment

##### Skin protection

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 EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Full contact

Material: butyl-rubber

Minimum layer thickness: 0.7 mm

Break through time: 480 min

Material tested: Butoject® (KCL 898)

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substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.4 mm

Break through time: 30 min

Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

### **Respiratory protection**

Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds

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.

required when vapours/aerosols are generated. Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

### **Control of environmental exposure**

Prevent product from entering drains.

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## **SECTION 9: Physical and chemical properties**

### **9.1 Information on basic physical and chemical properties**

a) Appearance	Form: liquid Color: yellow
b) Odor	characteristic
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/ range: 14 - 16 °C (57 - 61 °F) - lit.
f) Initial boiling point and boiling range	230 - 231 °C 446 - 448 °F - lit.
g) Flash point	98 °C (208 °F)
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	Lower explosion limit: 2.2 %(V)
k) Vapor pressure	0.2 hPa at 20 °C (68 °F)
l) Vapor density	4.74
m) Density	1.157 g/cm <sup>3</sup> at 25 °C (77 °F) - lit.

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	Relative density	No data available
n)	Water solubility	0.419 g/l at 20 °C (68 °F)
o)	Partition coefficient: n-octanol/water	log Pow: 2.5 - Bioaccumulation is not expected.
p)	Autoignition temperature	No data available
q)	Decomposition temperature	270 °C (518 °F) -
r)	Viscosity	No data available
s)	Explosive properties	No data available
t)	Oxidizing properties	none

## 9.2 Other safety information

Relative vapor density	4.74
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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

No data available

### 10.2 Chemical stability

No data available

### 10.3 Possibility of hazardous reactions

Risk of explosion with:

alkali salts

Peroxides

sulfuric acid

Sulfur trioxide

Reducing agents

Exothermic reaction with:

Ammonia

Sodium hydroxide

strong oxidising agents

Strong acids

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

### 10.4 Conditions to avoid

No data available

### 10.5 Incompatible materials

No data available

### 10.6 Hazardous decomposition products

In the event of fire: see section 5

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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - male and female - 1,784 mg/kg

(OECD Test Guideline 401)

Inhalation: No data available

Dermal: 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

No data available

#### Germ cell mutagenicity

Test Type: Mutagenicity (mammal cell test): chromosome aberration.

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 479

Result: negative

Test Type: Ames test

Test system: Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Test Type: unscheduled DNA synthesis assay

Species: Rat

Cell type: Liver cells

Application Route: Oral

Result: negative

Remarks: (ECHA)

#### 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**

May cause damage to organs through prolonged or repeated exposure.

**Aspiration hazard**

No data available

**11.2 Additional Information**

RTECS: XT2975000

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.

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**SECTION 12: Ecological information****12.1 Toxicity**

Toxicity to fish	flow-through test LC50 - Danio rerio (zebra fish) - 35.3 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 7.4 mg/l - 48 h Remarks: (ECHA)
Toxicity to algae	Growth inhibition ErC50 - Chlorella pyrenoidosa - 14 mg/l - 96 h (OECD Test Guideline 201)
Toxicity to bacteria	EC50 - Photobacterium phosphoreum - 3.95 mg/l - 15 min Remarks: (IUCLID)
Toxicity to fish(Chronic toxicity)	semi-static test NOEC - Oryzias latipes (Orange-red killifish) - 2 mg/l - 28 d Remarks: (ECHA)
Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity)	Reproduction Test NOEC - Daphnia magna (Water flea) - 0.5 mg/l - 21 d

**12.2 Persistence and degradability**

Biodegradability	aerobic - Exposure time 14 d Result: 2 % - Not readily biodegradable. (OECD Test Guideline 301C)
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**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 Endocrine disrupting properties

No data available

#### 12.7 Other adverse effects

No data available

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### SECTION 13: Disposal considerations

#### 13.1 Waste treatment methods

No data available

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### SECTION 14: Transport information

#### DOT (US)

UN number: 1664 Class: 6.1 Packing group: II  
Proper shipping name: Nitrotoluenes, liquid  
Reportable Quantity (RQ): 1000 lbs  
Poison Inhalation Hazard: No

#### IMDG

UN number: 1664 Class: 6.1 Packing group: II EMS-No: F-A, S-A  
Proper shipping name: NITROTOLUENES, LIQUID  
Marine pollutant : yes

#### IATA

UN number: 1664 Class: 6.1 Packing group: II  
Proper shipping name: Nitrotoluenes, liquid

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### SECTION 15: Regulatory information

#### CERCLA Reportable Quantity

Components	CAS-No.	Component RQ (lbs)	Calculated product RQ (lbs)
3-nitrotoluene	99-08-1	1000	1000

#### SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

## **SARA 302 Extremely Hazardous Substances Threshold Planning Quantity**

This material does not contain any components with a section 302 EHS TPQ.

**SARA 311/312 Hazards** : Acute Health Hazard

**SARA 313** : 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.

## **US State Regulations**

### **Massachusetts Right To Know**

3-nitrotoluene 99-08-1

### **Pennsylvania Right To Know**

3-nitrotoluene 99-08-1

### **Maine Chemicals of High Concern**

Product does not contain any listed chemicals

### **Vermont Chemicals of High Concern**

Product does not contain any listed chemicals

### **Washington Chemicals of High Concern**

Product does not contain any listed chemicals

## **The ingredients of this product are reported in the following inventories:**

TSCA : All substances listed as active on the TSCA inventory

### **TSCA list**

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

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## **SECTION 16: Other information**

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact [mlsbranding@sial.com](mailto:mlsbranding@sial.com).

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