

## SAFETY DATA SHEET

Version 6.6  
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 : 1,3-Dimethyl-2-nitrobenzene

Product Number : N28353

Brand : Aldrich

CAS-No. : 81-20-9

**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)**

Flammable liquids (Category 4), H227

Acute toxicity, Oral (Category 4), H302

Short-term (acute) aquatic hazard (Category 2), H401

Long-term (chronic) aquatic hazard (Category 2), H411

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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

H227

Combustible liquid.

H302

Harmful if swallowed.

H411

Toxic to aquatic life with long lasting effects.

Precautionary Statements

P210

Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.

P264

Wash skin thoroughly after handling.

P270

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

P273

Avoid release to the environment.

P280

Wear protective gloves/ eye protection/ face protection.

P301 + P312 + P330

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

P370 + P378

In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.

P391

Collect spillage.

P403 + P235

Store in a well-ventilated place. Keep cool.

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 : 2-Nitro-m-xylene

Formula :  $C_8H_9NO_2$

Molecular weight : 151.16 g/mol

CAS-No. : 81-20-9

EC-No. : 201-333-6

Component	Classification	Concentration
<b>2-Nitro-m-xylene</b>		
	Flam. Liq. 4; Acute Tox. 4; Aquatic Acute 2; Aquatic Chronic 2; H227, H302, 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**

Contains no substances with occupational exposure limit values.

### **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)

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)).

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: clear, liquid Color: yellow
b) Odor	aromatic
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	225 °C 437 °F at 992 hPa - lit.
g) Flash point	88 °C (190 °F) - closed cup
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	No data available
k) Vapor pressure	No data available
l) Vapor density	No data available
m) Density	1.112 g/cm <sup>3</sup> at 25 °C (77 °F) - lit.
Relative density	No data available
n) Water solubility	insoluble
o) Partition coefficient: n-octanol/water	log Pow: 2.95 - Bioaccumulation is not expected.
p) Autoignition temperature	No data available
q) Decomposition temperature	300 °C (572 °F) -
r) Viscosity	No data available
s) Explosive properties	No data available
t) Oxidizing properties	none

### 9.2 Other safety information

No data available

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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

Violent reactions possible with:  
Oxidizing agents

### 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 - 1,600 mg/kg

Remarks: The value is given based on a SAR/AAR approach using OECD Toolbox, DEREK, VEGA QSAR models (CAESAR models), etc.

Inhalation: No data available

Dermal: No data available

#### Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation  
(OECD Test Guideline 404)

#### Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation  
(OECD Test Guideline 405)

#### Respiratory or skin sensitization

No data available

#### Germ cell mutagenicity

Test Type: Ames test

Test system: Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

#### Carcinogenicity

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is

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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: ZE4686000

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.

Hazardous properties cannot be excluded but are unlikely when the product is handled appropriately.

The following applies to aromatic nitro compounds in general: systemic effect: methaemoglobinaemia with headache, cardiac dysrhythmias, drop in blood pressure, dyspnoea, and spasms; principal sign: cyanosis (blue discolouration of the blood).

Handle in accordance with good industrial hygiene and safety practice.

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## **SECTION 12: Ecological information**

### **12.1 Toxicity**

Toxicity to fish	LC50 - Pimephales promelas (fathead minnow) - 9.2 mg/l - 96 h Remarks: The value is given based on a SAR/AAR approach using OECD Toolbox, DEREK, VEGA QSAR models (CAESAR models), etc.
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Toxicity to daphnia and other aquatic invertebrates	LC50 - Daphnia magna (Water flea) - 9.2 mg/l - 48 h Remarks: The value is given based on a SAR/AAR approach using OECD Toolbox, DEREK, VEGA QSAR models (CAESAR models), etc.
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### **12.2 Persistence and degradability**

Biodegradability	Result: < 10 % - Not readily biodegradable. Remarks: (External MSDS)
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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**

Avoid release to the environment.

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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: 1665    Class: 6.1    Packing group: II  
Proper shipping name: Nitroxylenes, liquid  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

#### **IMDG**

UN number: 1665    Class: 6.1    Packing group: II EMS-No: F-A, S-A  
Proper shipping name: NITROXYLENES, LIQUID  
Marine pollutant : yes

#### **IATA**

UN number: 1665    Class: 6.1    Packing group: II  
Proper shipping name: Nitroxylenes, liquid

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## **SECTION 15: Regulatory information**

### **CERCLA Reportable Quantity**

This material does not contain any components with a CERCLA RQ.

### **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** : Fire 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**

No components are subject to the Massachusetts Right to Know Act.

### **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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