

## SAFETY DATA SHEET

Version 6.1  
Revision Date 05/25/2018  
Print Date 11/19/2018

### 1. PRODUCT AND COMPANY IDENTIFICATION

#### 1.1 Product identifiers

Product name : Nitromethane-d<sub>3</sub>

Product Number : 151963

Brand : Aldrich

CAS-No. : 13031-32-8

#### 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 Street  
ST. LOUIS MO 63103  
UNITED STATES

Telephone : +1 314 771-5765

Fax : +1 800 325-5052

#### 1.4 Emergency telephone number

Emergency Phone # : (314) 776-6555

### 2. HAZARDS IDENTIFICATION

#### 2.1 Classification of the substance or mixture

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

Flammable liquids (Category 3), H226

Acute toxicity, Oral (Category 4), H302

Acute toxicity, Inhalation (Category 3), H331

Carcinogenicity (Category 2), H351

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)

H226 : Flammable liquid and vapour.

H302 : Harmful if swallowed.

H331 : Toxic if inhaled.

H351	Suspected of causing cancer.
Precautionary statement(s)	
P201	Obtain special instructions before use.
P202	Do not handle until all safety precautions have been read and understood.
P210	Keep away from heat/sparks/open flames/hot surfaces. No smoking.
P233	Keep container tightly closed.
P240	Ground/bond container and receiving equipment.
P241	Use explosion-proof electrical/ ventilating/ lighting equipment.
P242	Use only non-sparking tools.
P243	Take precautionary measures against static discharge.
P261	Avoid breathing 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.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P312 + P330	IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell. Rinse mouth.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.
P304 + P340 + P311	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/doctor.
P308 + P313	IF exposed or concerned: Get medical advice/ attention.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
P403 + P235	Store in a well-ventilated place. Keep cool.
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 : Trideuteronitromethane

Molecular weight : 64.06 g/mol

CAS-No. : 13031-32-8

EC-No. : 235-892-2

#### Hazardous components

Component	Classification	Concentration
<b>Nitromethane-d3</b>		
	Flam. Liq. 3; Acute Tox. 4; Acute Tox. 3; Carc. 2; H226, H302, H331, H351	<= 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**

Do NOT induce vomiting. 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

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**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 (NO<sub>x</sub>)

**5.3 Advice for firefighters**

Wear self-contained breathing apparatus for firefighting if necessary.

**5.4 Further information**

Use water spray to cool unopened containers.

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**6. ACCIDENTAL RELEASE MEASURES****6.1 Personal precautions, protective equipment and emergency procedures**

Wear respiratory protection. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.  
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.

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

Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

**6.4 Reference to other sections**

For disposal see section 13.

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**7. HANDLING AND STORAGE****7.1 Precautions for safe handling**

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.  
Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.  
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. Containers which are opened must be carefully resealed and kept upright to prevent leakage.  
Store under inert gas. hygroscopic  
Storage class (TRGS 510): 3: Flammable liquids

**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
Nitromethane-d3	13031-32-8	TWA	20.000000 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Upper Respiratory Tract irritation Thyroid effects Lung damage Confirmed animal carcinogen with unknown relevance to humans		
		TWA	20 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Upper Respiratory Tract irritation Thyroid effects Lung damage Confirmed animal carcinogen with unknown relevance to humans		
		TWA	100.000000 ppm 250.000000 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		The value in mg/m3 is approximate.		
		See Appendix D - Substances with No Established RELs		
		PEL	2 ppm 5 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)

### 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.

##### Body Protection

Complete suit protecting against chemicals, Flame retardant antistatic protective clothing., 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 respirator with multi-purpose combination (US) or type ABEK (EN 14387) 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.

## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

- |                    |   |
|--------------------|---|
| a) Appearance      | Form: clear, liquid<br>Colour: colourless |
| b) Odour           | No data available                         |
| c) Odour Threshold | No data available                         |

d) pH	No data available
e) Melting point/freezing point	No data available
f) Initial boiling point and boiling range	100 °C (212 °F) - lit.
g) Flash point	35 °C (95 °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) Vapour pressure	36.4 hPa at 20 °C (68 °F)
l) Vapour density	No data available
m) Relative density	1.183 g/cm <sup>3</sup> at 25 °C (77 °F)
n) Water solubility	No data available
o) Partition coefficient: n-octanol/water	No data available
p) Auto-ignition temperature	No data available
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

No data available

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## 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

Vapours may form explosive mixture with air.

### 10.4 Conditions to avoid

Heat, flames and sparks.

### 10.5 Incompatible materials

Strong oxidizing agents

### 10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NO<sub>x</sub>)

Other decomposition products - No data available

In the event of fire: see section 5

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## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - 940 mg/kg

Remarks: (RTECS)

LD50 Dermal - Rabbit - > 2,000 mg/kg

Remarks: (IUCLID)

#### Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation

Remarks: (IUCLID)

#### Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation

Remarks: (IUCLID)

#### Respiratory or skin sensitisation

Sensitisation test: - Guinea pig

Result: negative

Remarks: (IUCLID)

#### Germ cell mutagenicity

Ames test

Result: negative

(IUCLID)

#### Carcinogenicity

IARC: 2B - Group 2B: Possibly carcinogenic to humans (Nitromethane-d3)

NTP: RAHC - Reasonably anticipated to be a human carcinogen (Nitromethane-d3)

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

##### Specific target organ toxicity - single exposure

##### Specific target organ toxicity - repeated exposure

##### Aspiration hazard

#### Additional Information

RTECS: Not available

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

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## 12. ECOLOGICAL INFORMATION

### 12.1 Toxicity

Toxicity to fish LC50 - Danio rerio (zebra fish) - 460 mg/l - 48 h(Nitromethane-d3)  
(OECD Test Guideline 203)

Toxicity to daphnia and other aquatic invertebrates EC50 - Daphnia magna (Water flea) - 450 mg/l - 24 h(Nitromethane-d3)  
(OECD Test Guideline 202)

Toxicity to algae IC50 - Desmodesmus subspicatus (green algae) - 36 mg/l - 72

h(Nitromethane-d3)  
(OECD Test Guideline 201)

Toxicity to bacteria      EC50 - Photobacterium phosphoreum - 5,621 mg/l - 30 min(Nitromethane-d3)  
Remarks: (Lit.)

## 12.2 Persistence and degradability

Biodegradability      Result: - Not readily biodegradable.

(OECD Test Guideline 301D)

## 12.3 Bioaccumulative potential

## 12.4 Mobility in soil

## 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

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# 13. DISPOSAL CONSIDERATIONS

## 13.1 Waste treatment methods

### Product

Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

### Contaminated packaging

Dispose of as unused product.

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# 14. TRANSPORT INFORMATION

## DOT (US)

UN number: 1261      Class: 3      Packing group: II  
Proper shipping name: Nitromethane  
Poison Inhalation Hazard: No

## IMDG

UN number: 1261      Class: 3      Packing group: II      EMS-No: F-E, S-D  
Proper shipping name: NITROMETHANE

## IATA

UN number: 1261      Class: 3      Packing group: II  
Proper shipping name: Nitromethane  
IATA Passenger: Not permitted for transport

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# 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

The following components are subject to reporting levels established by SARA Title III, Section 313:

	CAS-No.	Revision Date
Nitromethane-d3	13031-32-8	1993-04-24

## SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard, Chronic Health Hazard

## Massachusetts Right To Know Components

CAS-No.	Revision Date
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Nitromethane-d3	13031-32-8	1993-04-24
<b>Pennsylvania Right To Know Components</b>		
Nitromethane-d3	CAS-No. 13031-32-8	Revision Date 1993-04-24
<b>New Jersey Right To Know Components</b>		
Nitromethane-d3	CAS-No. 13031-32-8	Revision Date 1993-04-24
<b>California Prop. 65 Components</b>		
WARNING! This product contains a chemical known to the State of California to cause cancer.	CAS-No. 13031-32-8	Revision Date 2007-09-28
Nitromethane-d3		

## 16. OTHER INFORMATION

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

H226	Flammable liquid and vapour.
H302	Harmful if swallowed.
H331	Toxic if inhaled.
H351	Suspected of causing cancer.

### HMIS Rating

Health hazard:	1
Chronic Health Hazard:	*
Flammability:	3
Physical Hazard	0

### NFPA Rating

Health hazard:	3
Fire Hazard:	3
Reactivity Hazard:	0

### Further information

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### Preparation Information

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

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