SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name: Nitromethane-d₃

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 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 3), H226
Acute toxicity, Oral (Category 4), H302
Acute toxicity, Inhalation (Category 4), H332
Carcinogenicity (Category 2), H351
Reproductive toxicity (Category 2), H361

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

2.2 GHS Label elements, including precautionary statements

Pictogram
The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada.

### Signal Word

**Warning**

### Hazard statement(s)

- **H226** Flammable liquid and vapor.
- **H302 + H332** Harmful if swallowed or if inhaled.
- **H351** Suspected of causing cancer.
- **H361** Suspected of damaging fertility or the unborn child.

### 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 mist or vapors.
- **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 + P312** IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.
- **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 + 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

### SECTION 3: Composition/information on ingredients

#### 3.1 Substances

**Synonyms**: Trideuteronitromethane

**Formula**: CD3NO2
**Molecular weight**: 64.06 g/mol
**CAS-No.**: 13031-32-8
**EC-No.**: 235-892-2

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
</table>

Aldrich - 151963
SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice
Show this material safety data sheet to the doctor in attendance.

If inhaled
After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

In case of skin contact
In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/shower. Consult a physician.

In case of eye contact
After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed
After swallowing: immediately make victim drink water (two glasses at most). 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

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media
Water Foam Carbon dioxide (CO2) Dry powder

Unsuitable extinguishing media
For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture
Carbon oxides
Nitrogen oxides (NOx)
Combustible.
Vapors are heavier than air and may spread along floors.
Forms explosive mixtures with air at elevated temperatures.
Development of hazardous combustion gases or vapours possible in the event of fire.
5.3 **Advice for firefighters**
Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 **Further information**
Remove container from danger zone and cool with water. Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

**SECTION 6: Accidental release measures**

6.1 **Personal precautions, protective equipment and emergency procedures**
Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert. For personal protection see section 8.

6.2 **Environmental precautions**
Do not let product enter drains. Risk of explosion.

6.3 **Methods and materials for containment and cleaning up**
Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 **Reference to other sections**
For disposal see section 13.

**SECTION 7: Handling and storage**

7.1 **Precautions for safe handling**
**Advice on safe handling**
Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

**Advice on protection against fire and explosion**
Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

**Hygiene measures**
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance. 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
SECTION 8: Exposure controls/personal protection

8.1 Control parameters

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>nitro(2H3)methane</td>
<td>13031-32-8</td>
<td>TWA</td>
<td>20 ppm</td>
<td>USA. ACGIH Threshold Limit Values (TLV)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Remarks: Confirmed animal carcinogen with unknown relevance to humans</td>
</tr>
<tr>
<td></td>
<td></td>
<td>TWA</td>
<td>100 ppm 250 mg/m³</td>
<td>USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants</td>
</tr>
<tr>
<td></td>
<td></td>
<td>PEL</td>
<td>2 ppm 5 mg/m³</td>
<td>California permissible exposure limits for chemical contaminants (Title 8, Article 107)</td>
</tr>
</tbody>
</table>

8.2 Exposure controls

**Appropriate engineering controls**
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

**Personal protective equipment**

**Eye/face protection**
Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

**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).
Splash contact
Material: Viton®
Minimum layer thickness: 0.7 mm
Break through time: 120 min
Material tested: Vitoject® (KCL 890 / Aldrich Z677698, Size M)

**Body Protection**
Flame retardant antistatic protective clothing.

**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**
Do not let product enter drains. Risk of explosion.

---

### SECTION 9: Physical and chemical properties

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

<table>
<thead>
<tr>
<th>Property</th>
<th>Details</th>
</tr>
</thead>
<tbody>
<tr>
<td>Appearance</td>
<td>Form: clear, liquid</td>
</tr>
<tr>
<td></td>
<td>Color: colorless</td>
</tr>
<tr>
<td>Odor</td>
<td>No data available</td>
</tr>
<tr>
<td>Odor Threshold</td>
<td>No data available</td>
</tr>
<tr>
<td>pH</td>
<td>No data available</td>
</tr>
<tr>
<td>Melting point/freezing point</td>
<td>No data available</td>
</tr>
<tr>
<td>Initial boiling point and boiling range</td>
<td>100 °C 212 °F - lit.</td>
</tr>
<tr>
<td>Flash point</td>
<td>35 °C (95 °F) - closed cup</td>
</tr>
<tr>
<td>Evaporation rate</td>
<td>No data available</td>
</tr>
<tr>
<td>Flammability (solid, gas)</td>
<td>No data available</td>
</tr>
<tr>
<td>Upper/lower flammability or explosive limits</td>
<td>Upper explosion limit: 63 % (V)</td>
</tr>
<tr>
<td></td>
<td>Lower explosion limit: 7.1 % (V)</td>
</tr>
<tr>
<td>Vapor pressure</td>
<td>36.4 hPa at 20 °C (68 °F)</td>
</tr>
<tr>
<td>Vapor density</td>
<td>No data available</td>
</tr>
<tr>
<td>Density</td>
<td>1.183 g/cm³ at 25 °C (77 °F) - lit.</td>
</tr>
<tr>
<td>Relative density</td>
<td>No data available</td>
</tr>
<tr>
<td>Water solubility</td>
<td>No data available</td>
</tr>
<tr>
<td>Partition coefficient: n-octanol/water</td>
<td>No data available</td>
</tr>
<tr>
<td>Autoignition temperature</td>
<td>No data available</td>
</tr>
<tr>
<td>Decomposition temperature</td>
<td>No data available</td>
</tr>
<tr>
<td>Viscosity</td>
<td>No data available</td>
</tr>
<tr>
<td>Explosive properties</td>
<td>No data available</td>
</tr>
<tr>
<td>Oxidizing properties</td>
<td>none</td>
</tr>
</tbody>
</table>

#### 9.2 Other safety information
No data available
SECTION 10: Stability and reactivity

10.1 Reactivity
Vapor/air-mixtures are explosive at intense warming.

10.2 Chemical stability
The product is chemically stable under standard ambient conditions (room temperature).

10.3 Possibility of hazardous reactions
Exothermic reaction with:
- Hydrocarbons
- perchlorates
Risk of explosion with:
- anilines
- strong alkalis
- phosphoric acid
- Nitric acid
- Amines
- Heavy metals
- metallic oxides
- organic halides
- silver salt
- aluminium chloride
- formaldehyde
- alkali hydroxides
- Ammonia
- iodides
- Halogenated hydrocarbon acids
- Chloroform
- oxyhalogenic compounds
- Organic Substances
- Oxidizing agents
- Acetone
- powdered aluminium
- formic acid
- ammonium hydroxide bases
- calcium hypochlorite
- Sodium hydroxide
- lithium aluminium hydride
- sodium carbonate
- hydrides
- nitrous acid
- conc. sulfuric acid
- Potassium hydroxide
- Calcium hydroxide
- Morpholine
- Hydrazine hydrate
- with
- Methanol
formaldehyde
with
Air
Amines
with
Heavy metals
with
alkali hydroxides
Formation of explosive salts possible.
Violent reactions possible with:
Strong oxidizing agents

10.4 Conditions to avoid
Heating.

10.5 Incompatible materials
No data available

10.6 Hazardous decomposition products
In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity
LD50 Oral - Rat - male and female - 1,478 mg/kg
Remarks: (ECHA)
The value is given in analogy to the following substances: nitromethane
Symptoms: Nausea, Vomiting, Diarrhea
LC50 Inhalation - Rabbit - 4 h - 14.34 mg/l - vapor
Remarks: (ECHA)
The value is given in analogy to the following substances: nitromethane
LD50 Dermal - Rabbit - male and female - > 2,000 mg/kg
(OECD Test Guideline 402)
Remarks: The value is given in analogy to the following substances: nitromethane

Skin corrosion/irritation
Skin - Rabbit
Result: No skin irritation - 4 h
(OECD Test Guideline 404)
Remarks: The value is given in analogy to the following substances: nitromethane

Serious eye damage/eye irritation
Eyes - Rabbit
Result: No eye irritation
Remarks: (ECHA)
The value is given in analogy to the following substances: nitromethane

Respiratory or skin sensitization
Intracutaneous test - Guinea pig
Result: negative
Remarks: (ECHA)
The value is given in analogy to the following substances: nitromethane

**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
Remarks: The value is given in analogy to the following substances: nitromethane
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 473
Result: negative
Remarks: The value is given in analogy to the following substances: nitromethane

**Carcinogenicity**
Suspected of causing cancer.
IARC: 2B - Group 2B: Possibly carcinogenic to humans (nitro(2H3)methane)
NTP: RAHC - Reasonably anticipated to be a human carcinogen (nitro(2H3)methane)
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**
Suspected of damaging the unborn child.

**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**
Repeated dose toxicity - Rat - male and female - Oral - 28 Days - LOAEL (Lowest observed adverse effect level) - 100 mg/kg
Remarks: (ECHA)
The value is given in analogy to the following substances: nitromethane

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.
After absorption:

Methaemoglobinemia

Absorption may result in damage of the following:

Liver
Kidney

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

Stomach - Irregularities - Based on Human Evidence
Stomach - Irregularities - Based on Human Evidence

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish static test LC50 - Pimephales promelas (fathead minnow) - > 659.2 mg/l - 96 h (APHA 231)
Remarks: The value is given in analogy to the following substances: nitromethane

Toxicity to daphnia and other aquatic invertebrates static test EC50 - Daphnia magna (Water flea) - > 103 mg/l - 48 h (OECD Test Guideline 202)
Remarks: The value is given in analogy to the following substances: nitromethane

Toxicity to algae static test ErC50 - Pseudokirchneriella subcapitata (green algae) - > 102 mg/l - 72 h (OECD Test Guideline 201)
Remarks: The value is given in analogy to the following substances: nitromethane

Toxicity to bacteria static test EC50 - activated sludge - 310 mg/l - 30 min (OECD Test Guideline 209)
Remarks: The value is given in analogy to the following substances: 1-nitropropane

12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 28 d
Result: 9.9 % - Not readily biodegradable.
(OECD Test Guideline 301D)
Remarks: The value is given in analogy to the following substances:
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
Discharge into the environment must be avoided.

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product
Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

SECTION 14: Transport information

DOT (US)
UN number: 1261    Class: 3    Packing group: II
Proper shipping name: Nitromethane
Reportable Quantity (RQ):
    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

SECTION 15: Regulatory information

SARA 302 Components
This material does not contain any components with a section 302 EHS TPQ.
**SARA 313 Components**
The following components are subject to reporting levels established by SARA Title III, Section 313:

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>nitro(2H3)methane</td>
<td>13031-32-8</td>
<td>2013-02-08</td>
</tr>
</tbody>
</table>

**SARA 311/312 Hazards**
Fire Hazard, Acute Health Hazard, Chronic Health Hazard

**Massachusetts Right To Know Components**

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>nitro(2H3)methane</td>
<td>13031-32-8</td>
<td>2013-02-08</td>
</tr>
</tbody>
</table>

**Pennsylvania Right To Know Components**

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>nitro(2H3)methane</td>
<td>13031-32-8</td>
<td>2013-02-08</td>
</tr>
</tbody>
</table>

**California Prop. 65 Components**
, which is/are known to the State of California to cause cancer. For more information go to www.P65Warnings.ca.gov.nitro(2H3)methane

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>nitro(2H3)methane</td>
<td>13031-32-8</td>
<td>2007-09-28</td>
</tr>
</tbody>
</table>

**SECTION 16: Other information**

**Further information**
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.

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Details in analogy to the undeuterated compound.

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Version: 6.8 Revision Date: 08/27/2023 Print Date: 01/06/2024