

SAFETY DATA SHEET

Version 6.5
Revision Date 06/03/2022
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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
Carcinogenicity (Category 2), H351
Short-term (acute) aquatic hazard (Category 3), H402

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 statement(s)	
H226	Flammable liquid and vapor.
H302	Harmful if swallowed.
H351	Suspected of causing cancer.
H402	Harmful to aquatic life.
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.
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/ 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.
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

Component	Classification	Concentration
nitro(2H3)methane		
	Flam. Liq. 3; Acute Tox. 4; Carc. 2; Aquatic Acute 3; H226, H302, H351, H402	<= 100 %

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

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.

In case of skin contact

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

In case of eye contact

After eye contact: rinse out with plenty of water. 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

Carbon dioxide (CO₂) Dry powder

Unsuitable extinguishing media

Foam Water

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Nitrogen oxides (NO_x)

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

In the event of fire, wear self-contained breathing apparatus.

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. Chemisorb®). 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 protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures

Change contaminated clothing. Preventive skin protection recommended. Wash hands 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

Ingredients with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
nitro(2H3)methane	13031-32-8	TWA	20 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Confirmed animal carcinogen with unknown relevance to humans		

		TWA	100 ppm 250 mg/m ³	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		PEL	2 ppm 5 mg/m ³	California permissible exposure limits for chemical contaminants (Title 8, Article 107)

8.2 Exposure controls

Appropriate engineering controls

Change contaminated clothing. Preventive skin protection recommended. Wash hands 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 EN374 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

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

- | | |
|---------------------------------|----------------------|
| a) Appearance | Form: liquid |
| b) Odor | No data available |
| c) Odor Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | No data available |
| f) Initial boiling point | 100 °C 212 °F - lit. |

Aldrich - 151963

Page 5 of 10

and boiling range

g) Flash point	44 °C (111 °F)
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	Upper explosion limit: 63 %(V) Lower explosion limit: 7.1 %(V)
k) Vapor pressure	No data available
l) Vapor density	No data available
m) Density	1.183 g/cm ³ at 25 °C (77 °F) - lit.
Relative density	No data available
n) Water solubility	No data available
o) Partition coefficient: n-octanol/water	No data available
p) Autoignition 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

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

Aldrich - 151963

Page 6 of 10

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.

10.4 Conditions to avoid

Heating.

10.5 Incompatible materials

various plastics

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 - 940 mg/kg

Remarks: (RTECS)

Inhalation: No data available

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 sensitization

Sensitisation test: - Guinea pig

Result: negative

Remarks: (IUCLID)

Germ cell mutagenicity

Test Type: Ames test

Result: negative

Remarks: (IUCLID)

Carcinogenicity

IARC: 2B - Group 2B: Possibly carcinogenic to humans (nitro(2H3)methane)

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

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

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish	LC50 - Danio rerio (zebra fish) - 460 mg/l - 48 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	EC50 - Daphnia magna (Water flea) - 450 mg/l - 24 h (OECD Test Guideline 202)
Toxicity to algae	IC50 - Desmodesmus subspicatus (green algae) - 36 mg/l - 72 h (OECD Test Guideline 201)
Toxicity to bacteria	EC50 - Photobacterium phosphoreum - 5,621 mg/l - 30 min Remarks: (Lit.)

12.2 Persistence and degradability

Biodegradability Result: - Not readily biodegradable.

(OECD Test Guideline 301D)

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

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. See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14: Transport information

DOT (US)

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

Aldrich - 151963

Page 9 of 10

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:

nitro(2H3)methane	CAS-No. 13031-32-8	Revision Date 2013-02-08
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SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

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

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: 6.5

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