

SAFETY DATA SHEET

Version 6.3
Revision Date 02/18/2021
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SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifiers**

Product name : N-Desmethyloclobazam-13C6

Product Number : D-128
Brand : Cerilliant
Index-No. : 608-001-00-3

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 2), H225
Acute toxicity, Oral (Category 4), H302
Acute toxicity, Inhalation (Category 4), H332
Acute toxicity, Dermal (Category 4), H312
Eye irritation (Category 2A), H319

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)	
H225	Highly flammable liquid and vapor.
H302 + H312 + H332	Harmful if swallowed, in contact with skin or if inhaled.
H319	Causes serious eye irritation.
Precautionary statement(s)	
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/ vapors/ 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/ 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.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P337 + P313	If eye irritation persists: Get medical advice/ attention.
P363	Wash contaminated clothing before reuse.
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.
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

3.2 Mixtures

Molecular weight : 41.05 g/mol

Component		Classification	Concentration
Acetonitrile			
CAS-No.	75-05-8	Flam. Liq. 2; Acute Tox. 4; Eye Irrit. 2A; H225, H302, H332, H312, H319	>= 90 - <= 100 %
EC-No.	200-835-2		
Index-No.	608-001-00-3		
Registration number	01-2119471307-38-XXXX		

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. If breathing stops: mouth-to-mouth breathing or artificial respiration. Oxygen if necessary. Immediately call in physician.

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 (NO_x)

Combustible.

Pay attention to flashback.

Vapors are heavier than air and may spread along floors.

Development of hazardous combustion gases or vapours possible in the event of fire.

Forms explosive mixtures with air at ambient temperatures.

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. 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 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

Storage conditions

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

Storage stability

Recommended storage temperature
-20 °C

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

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
Acetonitrile	75-05-8	TWA	20 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Not classifiable as a human carcinogen Danger of cutaneous absorption		
		TWA	20 ppm 34 mg/m3	USA. NIOSH Recommended Exposure Limits
		TWA	40 ppm 70 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		The value in mg/m3 is approximate.		
		PEL	40 ppm 70 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		
		STEL	60 ppm 105 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		
		TWA	40 ppm 70 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		STEL	60 ppm 105 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000

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

required

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: clear, liquid Color: colorless
b) Odor	ether-like
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/range: -47.99 °C (-54.38 °F)
f) Initial boiling point and boiling range	81.0 - 82.0 °C 177.8 - 179.6 °F at 1013.3 hPa
g) Flash point	2.0 °C (35.6 °F) - closed cup
h) Evaporation rate	5.8
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	Upper explosion limit: 16 %(V) Lower explosion limit: 3 %(V)
k) Vapor pressure	73.18 hPa at 15 °C (59 °F) 121.44 hPa at 25 °C(77 °F) 413.23 hPa at 55 °C(131 °F) 98.64 hPa at 20 °C(68 °F)
l) Vapor density	1.42 - (Air = 1.0)
m) Relative density	No data available
n) Water solubility	completely soluble
o) Partition coefficient: n-octanol/water	log Pow: -0.539 at 25 °C (77 °F)
p) Autoignition temperature	524.0 °C (975.2 °F)
q) Decomposition temperature	No data available
r) Viscosity	No data available
s) Explosive properties	Not explosive
t) Oxidizing properties	The substance or mixture is not classified as oxidizing.

9.2 Other safety information

Surface tension	29.0 mN/m at 20.0 °C (68.0 °F)
Relative vapor density	1.42 - (Air = 1.0)

SECTION 10: Stability and reactivity

10.1 Reactivity

Vapors may form explosive mixture with air.

10.2 Chemical stability

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

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

Warming.

10.5 Incompatible materials

Strong oxidizing agents

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Mixture

Acute toxicity

Symptoms: Possible symptoms:, mucosal irritations

No data available

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

Mixture causes serious eye irritation.

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

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

Acute inhalation toxicity - Possible symptoms:, mucosal irritations

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

Not available

Treat as cyanide poisoning., Always have on hand a cyanide first-aid kit, together with proper instructions., The onset of symptoms is generally delayed pending conversion to cyanide., Nausea, Vomiting, Diarrhea, Headache, Dizziness, Rash, Cyanosis, excitement, depression, Drowsiness, impaired judgment, Lack of coordination, stupor, death

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

Components**Acetonitrile****Acute toxicity**

LD50 Oral - Mouse - male and female - 617 mg/kg

(OECD Test Guideline 401)

LC50 Inhalation - Mouse - male and female - 4 h - 6.022 mg/l

(OECD Test Guideline 403)

Acute toxicity estimate Dermal - 1,500 mg/kg

(Expert judgment)

Dermal: No data available

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: Causes serious eye irritation.

(OECD Test Guideline 405)

Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Respiratory or skin sensitization

Buehler Test - Guinea pig

Result: negative

(OECD Test Guideline 406)

Germ cell mutagenicity

Ames test

S. typhimurium

Result: negative

Remarks:

(ECHA)

In vitro mammalian cell gene mutation test
Chinese hamster ovary cells
Result: negative
Mutagenicity (mammal cell test): chromosome aberration.
Chinese hamster ovary cells
Result: Positive results were obtained in some in vitro tests.
Remarks:
(National Toxicology Program)
sister chromatid exchange assay
Chinese hamster ovary cells
Result: negative
Remarks:
Sister chromatid exchange
Saccharomyces cerevisiae
Result: positive
Remarks:
Cytogenetic analysis
(ECHA)
In vitro mammalian cell gene mutation test
Mouse lymphoma test
Result: negative
OECD Test Guideline 474
Mouse - male and female
Result: negative

Carcinogenicity

No evidence of carcinogenicity in animal studies.

Reproductive toxicity

Animal testing did not show any effects on fertility.

Specific target organ toxicity - single exposure

The substance or mixture is not classified as specific target organ toxicant, single exposure.

Specific target organ toxicity - repeated exposure

The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

Aspiration hazard

No aspiration toxicity classification

SECTION 12: Ecological information

12.1 Toxicity

Mixture

No data available

12.2 Persistence and degradability

No data available

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

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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

No data available

Components

Acetonitrile

Toxicity to fish	flow-through test LC50 - Pimephales promelas (fathead minnow) - 1,640 mg/l - 96 h Remarks: (ECHA)
Toxicity to algae	static test NOEC - Phaeodactylum tricornutum - 400 mg/l - 72 h (ISO 10253) static test ErC50 - Phaeodactylum tricornutum - 9,696 mg/l - 72 h (ISO 10253)
Toxicity to bacteria	

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Waste material must be disposed of in accordance with the national and local No mixing with other waste. Handle uncleaned containers like the product 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: 1648 Class: 3 Packing group: II
Proper shipping name: AcetonitrileSOLUTION

Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG

UN number: 1648 Class: 3 Packing group: II EMS-No: F-E, S-D
Proper shipping name: ACETONITRILESOLUTION

IATA

UN number: 1648 Class: 3 Packing group: II
Proper shipping name: AcetonitrileSOLUTION

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:

	CAS-No.	Revision Date
Acetonitrile	75-05-8	2007-07-01

SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard

Massachusetts Right To Know Components

	CAS-No.	Revision Date
Acetonitrile	75-05-8	2007-07-01

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

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Acetonitrile	75-05-8	2007-07-01

New Jersey Right To Know Components

	CAS-No.	Revision Date
Acetonitrile	75-05-8	2007-07-01

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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