SAFETY DATA SHEET

Version 8.0
Revision Date 03/05/2025
Print Date 03/14/2025

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

1.1 Product identifiers

Product name : Butonitazene-13C6 HCl

Product Number : B-114
Brand : Cerilliant

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 : Cerilliant Corporation
811 Paloma Drive, Suite A
ROUND ROCK TX 78665
UNITED STATES

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 3), H301
Acute toxicity, Inhalation (Category 3), H331
Acute toxicity, Dermal (Category 3), H311
Specific target organ toxicity - single exposure (Category 1), Eyes, Central nervous system, H370

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

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 Statements

H225	Highly flammable liquid and vapor.
H301 + H311 + H331	Toxic if swallowed, in contact with skin or if inhaled.
H370	Causes damage to organs (Eyes, Central nervous system).

Precautionary Statements

P210	Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P233	Keep container tightly closed.
P240	Ground and bond container and receiving equipment.
P241	Use explosion-proof electrical/ ventilating/ lighting/ equipment.
P242	Use non-sparking tools.
P243	Take action to prevent static discharges.
P260	Do not breathe 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 + P310 + P330	IF SWALLOWED: Immediately call a POISON CENTER/ doctor. 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.
P361 + P364	Take off immediately all contaminated clothing and wash it before reuse.
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

SECTION 3: Composition/information on ingredients

3.2 Mixtures

Component	Classification	Concentration

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

Methanol			
CAS-No. EC-No. Index-No. Registration number	67-56-1 200-659-6 603-001-00-X 01-2119433307-44-XXXX	Flam. Liq. 2; Acute Tox. 3; STOT SE 1; H225, H301, H331, H311, H370 Concentration limits: >= 10 %: STOT SE 1, H370; 3 - < 10 %: STOT SE 2, H371;	>= 80 - <= 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
First aiders need to protect themselves. 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. Call a physician immediately.

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

If swallowed
After swallowing: fresh air. Make victim drink ethanol (e.g. 1 drinking glass of a 40% alcoholic beverage). Call a doctor immediately (mention methanol ingestion). Only in exceptional cases, if no medical care is available within one hour, induce vomiting (only in fully conscious persons) and make victim drink ethanol again (approx. 0.3 ml of a 40% alcoholic beverage/kg body weight/hour).

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

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

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
Mixture with combustible ingredients.
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. 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 carefully 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.

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

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. Keep locked up or in an area accessible only to qualified or authorized persons.
Storage stability Recommended storage temperature
-25 - -10 °C
Storage class
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
Methanol	67-56-1	TWA	200 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Danger of cutaneous absorption		
		STEL	250 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Danger of cutaneous absorption		
		ST	250 ppm 325 mg/m3	USA. NIOSH Recommended Exposure Limits
		Potential for dermal absorption		
		TWA	200 ppm 260 mg/m3	USA. NIOSH Recommended Exposure Limits
		Potential for dermal absorption		
		TWA	200 ppm 260 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		PEL	200 ppm 260 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		
		C	1,000 ppm	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		

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

		STEL	250 ppm 325 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		

Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
Methanol	67-56-1	Methanol	15 mg/l	Urine	ACGIH - Biological Exposure Indices (BEI)
	Remarks	End of shift (As soon as possible after exposure ceases)			

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
Recommended Filter type: Filter type ABEK
The entrepeneur 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

a)	Appearance	Form: liquid
b)	Odor	No data available
c)	Odor Threshold	No data available

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

d)	pH	No data available
e)	Melting point/freezing point	No data available
f)	Initial boiling point and boiling range	No data available
g)	Flash point	9.7 °C (49.5 °F) - closed cup - Regulation (EC) No. 440/2008, Annex, A.9
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	No data available
	Relative density	No data available
n)	Water solubility	soluble
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
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

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

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
Oral: No data available
Inhalation: No data available
Dermal: No data available

Skin corrosion/irritation
No data available

Serious eye damage/eye irritation
No data available

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
Mixture causes damage to organs. - Eyes, Central nervous system

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

11.2 Additional Information

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

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

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

Components

Methanol

Acute toxicity
Acute toxicity estimate Oral - 100.1 mg/kg
(Expert judgment)
Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)
Symptoms: Nausea, Vomiting
Acute toxicity estimate Inhalation - 4 h - 3.1 mg/l - vapor
(Expert judgment)
Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)
Symptoms: Irritation symptoms in the respiratory tract.
Acute toxicity estimate Dermal - 300.1 mg/kg
(Expert judgment)
Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Skin corrosion/irritation
Skin - Rabbit
Result: No skin irritation
Remarks: (ECHA)
Remarks: Drying-out effect resulting in rough and chapped skin.

Serious eye damage/eye irritation
Eyes - Rabbit
Result: No eye irritation
Remarks: (ECHA)

Respiratory or skin sensitization
Sensitisation test: - Guinea pig
Result: negative
(OECD Test Guideline 406)

Germ cell mutagenicity
Based on available data the classification criteria are not met.
Test Type: Ames test
Test system: Salmonella typhimurium
Result: negative
Test Type: In vitro mammalian cell gene mutation test
Test system: Chinese hamster lung cells
Result: negative
Method: OECD Test Guideline 474
Species: Mouse - male and female - Bone marrow
Result: negative

Carcinogenicity
Did not show carcinogenic effects in animal experiments.

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

Reproductive toxicity
Based on available data the classification criteria are not met.

Specific target organ toxicity - single exposure
Causes damage to organs. - Eyes, Central nervous system
Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)
Acute oral toxicity - Nausea, Vomiting
Acute inhalation toxicity - Irritation symptoms in the respiratory tract.

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

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

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

Components

Methanol

Toxicity to fish	flow-through test LC50 - Lepomis macrochirus (Bluegill) - 15,400.0 mg/l - 96 h (US-EPA)
Toxicity to daphnia and other aquatic invertebrates	semi-static test EC50 - Daphnia magna (Water flea) - 18,260 mg/l - 96 h (OECD Test Guideline 202)
Toxicity to algae	static test ErC50 - Pseudokirchneriella subcapitata (green algae) - ca. 22,000.0 mg/l - 96 h (OECD Test Guideline 201)

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

Toxicity to bacteria	static test IC50 - activated sludge - > 1,000 mg/l - 3 h (OECD Test Guideline 209)
Toxicity to fish(Chronic toxicity)	NOEC - Oryzias latipes (Orange-red killifish) - 7,900 mg/l - 200 h Remarks: (External MSDS)

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: 1230 Class: 3 Packing group: II
Proper shipping name: MethanolSOLUTION

Reportable Quantity (RQ): 5000 lbs
Poison Inhalation Hazard: No

IMDG
UN number: 1230 Class: 3 (6.1) Packing group: II EMS-No: F-E, S-D
Proper shipping name: METHANOLSOLUTION

IATA
UN number: 1230 Class: 3 (6.1) Packing group: II
Proper shipping name: MethanolSOLUTION

SECTION 15: Regulatory information

CERCLA Reportable Quantity

Components	CAS-No.	Component RQ (lbs)	Calculated product RQ (lbs)
Methanol	67-56-1	5000	5000

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

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

Methanol	67-56-1	>= 90 - <= 100 %

Clean Air Act

This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).
The following chemical(s) are listed as HAP under the U.S. Clean Air Act, Section 112 (40 CFR 61):

Methanol	67-56-1	>= 90 - <= 100 %

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F).
The following chemical(s) are listed under the U.S. Clean Air Act Section 111 SOCMI Intermediate or Final VOC's (40 CFR 60.489):

Methanol	67-56-1	>= 90 - <= 100 %

Clean Water Act

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.
This product does not contain any Hazardous Chemicals listed under the U.S. CleanWater Act, Section 311, Table 117.3.
This product does not contain any toxic pollutants listed under the U.S. Clean Water Act Section 307
This product does not contain any priority pollutants related to the U.S. Clean Water Act

US State Regulations

Massachusetts Right To Know

Methanol	67-56-1

Pennsylvania Right To Know

Methanol	67-56-1

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

California Prop. 65

WARNING: This product can expose you to chemicals including Methanol, which is/are known to the State of California to cause birth defects or other reproductive harm. For more information go to www.P65Warnings.ca.gov.

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

The ingredients of this product are reported in the following inventories:

TSCA : Product contains substance(s) not listed on 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.

SECTION 16: Other information

Further information

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. 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.

Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

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.

Version: 8.0 Revision Date: 03/05/2025 Print Date: 03/14/2025

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