

SAFETY DATA SHEET

Version 6.3 Revision Date 05/03/2021 Print Date 09/08/2021

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

1.1 Product identifiers

Product name : Benzoylecgonine-D₈ solution

Product Number : B-014 Brand : Cerilliant

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 3), H301 Acute toxicity, Inhalation (Category 3), H331 Acute toxicity, Dermal (Category 3), H311

Specific target organ toxicity - single exposure (Category 1), H370

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.

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Millipore SigMa

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H301 + H311 + H331 H370	Toxic if swallowed, in contact with skin or if inhaled. Causes damage to organs.
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.
P260	Do not breathe dust/ fume/ gas/ mist/ vapors/ spray.
P264 P270	Wash skin thoroughly after handling.
P270 P271	Do not eat, drink or smoke when using this product. Use only outdoors or in a well-ventilated area.
P280	Wear protective gloves/ protective clothing/ eye protection/ face
1 200	protection.
P301 + P310	IF SWALLOWED: Immediately call a POISON CENTER/ doctor.
P303 + P361 + P353	IF ON SKIN (or hair): Remove/ Take off immediately all
. 555 / 1552 / 1555	contaminated clothing. Rinse skin with water/ shower.
P304 + P340	IF INHALED: Remove victim to fresh air and keep at rest in a
	position comfortable for breathing.
P307 + P311	IF exposed: Call a POISON CENTER or doctor/ physician.
P322	Specific measures (see supplemental first aid instructions on
	this label).
P330	Rinse mouth.
P361	Remove/ Take off immediately all contaminated clothing.
P363	Wash contaminated clothing before reuse.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant
	foam for extinction.
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

Molecular weight : 297.38 g/mol

Component		Classification	Concentration
Methanol			
CAS-No.	67-56-1	Flam. Liq. 2; Acute Tox. 3;	>= 90 - <=
EC-No.	200-659-6	STOT SE 1; H225, H301,	100 %
Index-No.	603-001-00-X	H331, H311, H370	
Registration	01-2119433307-44-	Concentration limits:	
number	XXXX	>= 10 %: STOT SE 1,	
		H370; 3 - < 10 %: STOT	
		SE 2, H371;	



Benzoylecgonine-D8			
CAS-No.	205446-21-5	Acute Tox. 3; H301	>= 0.1 - < 1 %

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

Consult a physician. Show this material safety data sheet to the doctor in attendance.

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

SECTION 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

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.



SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Wear respiratory protection. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapors accumulating to form explosive concentrations. Vapors 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 wetbrushing and place in container for disposal according to local regulations (see section 13).

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

Avoid contact with skin and eyes. Avoid inhalation of vapor or mist.

Advice on protection against fire and explosion

Use explosion-proof equipment. **Advice on protection against fire and explosion**Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

Hygiene measures

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

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. Containers which are opened must be carefully resealed and kept upright to prevent leakage. Store under inert gas. hygroscopic

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

ingreaterits with	workplace	control par	ameters	
Component	CAS-No.	Value	Control	Basis
			parameters	
Methanol	67-56-1	TWA	200 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Danger of o	cutaneous absor	,
	Remarks	STEL	250 ppm	USA. ACGIH Threshold Limit
				Values (TLV)
		Danger of o	cutaneous absor	ption
		TWA	200 ppm 260 mg/m3	USA. NIOSH Recommended Exposure Limits
		Potential fo	r dermal absorp	
		ST	250 ppm 325 mg/m3	USA. NIOSH Recommended Exposure Limits
		Potential fo	r dermal absorp	
		TWA	200 ppm	USA. Occupational Exposure
		1 447.1	260 mg/m3	Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		STEL	250 ppm 325 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		Skin notation	on	
		TWA	200 ppm 260 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		Skin notation	on	
		С	1,000 ppm	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		
		PEL	200 ppm 260 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		
		STEL	250 ppm 325 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article
				107)

Biological occupational exposure limits

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 exp	osure ceases)

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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.

Full contact

Material: butyl-rubber

Minimum layer thickness: 0.3 mm Break through time: 480 min

Material tested:Butoject® (KCL 897 / Aldrich Z677647, Size M)

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.4 mm Break through time: 30 min

Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail

sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

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.



SECTION 9: Physical and chemical properties

Information on basic physical and chemical properties 9.1

Form: liquid a) Appearance

b) Odor No data available

c) Odor Threshold No data available

No data available d) pH

e) Melting No data available point/freezing point

f) Initial boiling point and boiling range

64 - 65 °C 147 - 149 °F at 1.013 hPa

g) Flash point 9.7 °C (49.5 °F) - closed cup

h) Evaporation rate No data available No data available

Flammability (solid, i)

gas)

Upper/lower Upper explosion limit: 36 %(V) i) flammability or Lower explosion limit: 6 %(V) explosive limits

k) Vapor pressure No data available Vapor density No data available I) m) Relative density No data available No data available n) Water solubility

o) Partition coefficient: n-octanol/water

No data available

p) Autoignition No data available temperature

q) Decomposition temperature

No data available

No data available Viscosity r) s) Explosive properties No data available No data available Oxidizing properties

9.2 Other safety information

No data available

SECTION 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

No data available

10.4 Conditions to avoid

Heat, flames and sparks. Extremes of temperature and direct sunlight.

10.5 Incompatible materials

Acids, Oxidizing agents, Alkali metals, Strong oxidizing agents, Strong acids, Acid chlorides, Acid anhydrides, Reducing agents, Strong reducing agents, Phosphorus halides

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

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.

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.

ACGIH: No ingredient of this product present at levels greater than or equal to 0.1% is

identified as a carcinogen or potential carcinogen by ACGIH.

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.

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.

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

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

Components

Methanol

Acute toxicity

Acute toxicity estimate Oral - 100.1 mg/kg

(Expert judgment)

Symptoms: Nausea, Vomiting

Acute toxicity estimate Inhalation - 4 h - 3.1 mg/l

(Expert judgment)

Symptoms: Irritation symptoms in the respiratory tract.

Acute toxicity estimate Dermal - 300.1 mg/kg

(Expert judgment)

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation Remarks: (ECHA)

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.

Ames test

Salmonella typhimurium

Result: negative

In vitro mammalian cell gene mutation test

Chinese hamster lung cells

Result: negative

OECD Test Guideline 474

Mouse - male and female - Bone marrow

Result: negative

Carcinogenicity

Did not show carcinogenic effects in animal experiments.

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

Benzoylecgonine-D8

Acute toxicity

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

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

No data available

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

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 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

semi-static test EC50 - Daphnia magna (Water flea) - 18,260

and other aquatic

mg/l - 96 h

invertebrates

(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)

Toxicity to bacteria

static test IC50 - activated sludge - > 1,000 mg/l - 3 h

(OECD Test Guideline 209)

Benzoylecgonine-D8

No data available

SECTION 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.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

DOT (US)

UN number: 1230 Class: 3 Packing group: II

Proper shipping name: MethanolSOLUTION

Reportable Quantity (RQ): 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

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II:DDDB

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IATA

UN number: 1230 Class: 3 (6.1) Packing group: II

Proper shipping name: MethanolSOLUTION

SECTION 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
Methanol	67-56-1	2007-07-01

Massachusetts Right To Know Components

	CAS-No.	Revision Date
Methanol	67-56-1	2007-07-01

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

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Pennsylvania Right To Know Components Methanol	CAS-No. 67-56-1	Revision Date 2007-07-01
Methanol	CAS-No. 67-56-1	Revision Date 2007-07-01
New Jersey Right To Know Components Methanol	CAS-No. 67-56-1	Revision Date 2007-07-01
California Prop. 65 Components WARNING: This product contains a chemical known in the State of California to cause birth defects or other reproductive harm. Methanol	CAS-No. 67-56-1	Revision Date 2012-03-16

SECTION 16: Other information

Further information

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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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