

Printing date 12/07/2022

Revision date 12/07/2022

Page 1/11

## **1** Identification

- · Product identifier
- · Trade name: Benzoylecgonine-d3 (CRM)
- · Article number: 20860
- **Application of the substance / the mixture** This product is for research use - Not for human or veterinary diagnostic or therapeutic use.
- · Details of the supplier of the safety data sheet
- **Manufacturer/Supplier:** Cayman Chemical Co. 1180 E. Ellsworth Rd. Ann Arbor, MI 48108 USA
- Information department: Product safety department
   Emergency telephone number: During normal opening times: +1 (734) 971-3335 US/CANADA: 800-424-9300 Outside US/CANADA: 703-741-5970

## 2 Hazard(s) identification

25 Highly flammable liquid and vapor.
01 Toxic if swallowed.
11 Toxic in contact with skin.
31 Toxic if inhaled.
70 Causes damage to the central nervou system and the visual organs.
3

Printing date 12/07/2022

Revision date 12/07/2022

## Trade name: Benzoylecgonine-d3 (CRM)

	(Contd. from page 1)
· Label elements	5
· GHS label elem	-
The product is o	classified and labeled according to the Globally Harmonized System (GHS).
<ul> <li>Hazard pictogr</li> </ul>	rams
<u>e</u> 3	
GHS02 GHS	06 GHS08
01002 01100	
• Signal word Da	anger
· Hazard-determ	ining components of labeling:
Methanol	
<ul> <li>Hazard statem</li> </ul>	
H225	Highly flammable liquid and vapor.
	331 Toxic if swallowed, in contact with skin or if inhaled.
H370	Causes damage to the central nervous system and the visual organs.
<ul> <li>Precautionary P210</li> </ul>	Keep away from heat/sparks/open flames/hot surfaces No smoking.
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	Wash 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 P301+P310	Wear protective gloves/protective clothing/eye protection/face protection. If swallowed: Immediately call a poison center/doctor.
P321	Specific treatment (see on this label).
P330	Rinse mouth.
	53 If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with
	water/shower.
P304+P340	IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P307+P311	IF exposed: Call a POISON CENTER or doctor/physician.
P312	Call a poison center/doctor if you feel unwell.
P361+P364	Take off immediately all contaminated clothing and wash it before reuse.
P370+P378 P403+P233	In case of fire: Use CO2, powder or water spray to extinguish. 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 in accordance with local/regional/national/international
	regulations.
<ul> <li>Classification s</li> </ul>	
<ul> <li>NFPA ratings (</li> </ul>	scale 0 - 4)
Ha Ha	ealth = 0
	re = 3
	eactivity = 0
$\checkmark$	-
• HMIS-ratings (	scale 0 - 4)
HEALTH <b>*</b> 0 H	lealth = *0
	ire = 3
REACTIVITY 0 R	Reactivity = 0
	(Contd. on page 3)

US

Printing date 12/07/2022

Revision date 12/07/2022

(Contd. from page 2)

99.99%

0.01%

### Trade name: Benzoylecgonine-d3 (CRM)

- · Other hazards
- Results of PBT and vPvB assessment
- **PBT:** Not applicable.
- · **vPvB:** Not applicable.

## **3** Composition/information on ingredients

· Chemical characterization: Mixtures

· Description: Mixture of the substances listed below with nonhazardous additions.

- · Dangerous components:
- CAS: 67-56-1 Methanol
- RTECS: PC1400000

Other ingredients

115732-68-8 Benzoylecgonine-d3

## **4 First-aid measures**

### · Description of first aid measures

General information:

Immediately remove any clothing soiled by the product.

Remove breathing apparatus only after contaminated clothing have been completely removed.

In case of irregular breathing or respiratory arrest provide artificial respiration.

### · After inhalation:

Supply fresh air or oxygen; call for doctor.

In case of unconsciousness place patient stably in side position for transportation.

- After skin contact: Immediately wash with water and soap and rinse thoroughly.
- After eye contact: Rinse opened eye for several minutes under running water. Then consult a doctor.
- After swallowing: Do not induce vomiting; immediately call for medical help.
- · Information for doctor:
- · Most important symptoms and effects, both acute and delayed

May cause anemia, cough, CNS depression, drowsiness, headache, heart damage, lassitude (weakness, exhaustion), liver damage, narcosis, reproductive effects, teratogenic effects. No further relevant information available.

• Indication of any immediate medical attention and special treatment needed No further relevant information available.

## **5** Fire-fighting measures

- · Extinguishing media
- · Suitable extinguishing agents:

CO2, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam. • Special hazards arising from the substance or mixture

67-56-1During heating or in case of fire poisonous gases are produced.

- Advice for firefighters
- · Protective equipment: Mouth respiratory protective device.

(Contd. on page 4)

Printing date 12/07/2022

Revision date 12/07/2022

## Trade name: Benzoylecgonine-d3 (CRM)

(Contd. from page 3)

Wear protective equipment. Keep unprotected persons away.         Environmental precautions:         Dilute with plenty of water.         Do not allow to enter severs/ surface or ground water.         Methods and material for containment and cleaning up:         Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust).         Dispose contaminated material as waste according to item 13.         Ensure adequate ventilation.         Reference to other sections         See Section 7 for information on safe handling.         See Section 8 for information on personal protection equipment.         See Section 8 for information on personal protection equipment.         See Section 8 for information.         Protective Action Criteria for Chemicals         PAC-1:         67-56-1 [Methanol       2,100 pr         PAC-3:         67-56-1 [Methanol       7200* pr         Precautions for safe handling         Precautions for safe handling         Precautions for safe handling         Precautions for safe handling.         Precautions for safe handling.         Precaution of aerosols.         Information of aerosols.         Information of aerosols.         Information of aerosols.         Information about protection against explosions and fires: <th>Personal precautions, protective equipment and emergency proc Mount respiratory protective device.</th> <th>cedures</th>	Personal precautions, protective equipment and emergency proc Mount respiratory protective device.	cedures
Environmental precautions: Dilute with plenty of water. Do not allow to enter sewers/ surface or ground water. Methods and material for containment and cleaning up: Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust). Dispose contaminated material as waste according to item 13. Ensure adequate ventilation. Reference to other sections See Section 7 for information on safe handling. See Section 8 for information on personal protection equipment. See Section 13 for disposal information. Protective Action Criteria for Chemicals PAC-1: 67-56-1 [Methanol		
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PAC-2:       2,100 pp         67-56-1       Methanol       2,100 pp         PAC-3:       7200* pp         67-56-1       Methanol       7200* pp         Handling and storage         Handling:         Precautions for safe handling         Ensure good ventilation/exhaustion at the workplace.       Open and handle receptacle with care.         Prevent formation of aerosols.       Information about protection against explosions and fires:         Keep ignition sources away - Do not smoke.       Keep ignition sources away - Do not smoke.	67-56-1 Methanol	530 ppm
67-56-1       Methanol       2,100 pp         PAC-3:       67-56-1       Methanol       7200* pp         Handling and storage       7200* pp       7200* pp         Handling:       Precautions for safe handling       7200* pp         Ensure good ventilation/exhaustion at the workplace.       0pen and handle receptacle with care.       7200* pp         Prevent formation of aerosols.       Information about protection against explosions and fires:       Keep ignition sources away - Do not smoke.		
PAC-3:       67-56-1       Methanol       7200* pr         Handling and storage       7200* pr         Handling:       Precautions for safe handling         Ensure good ventilation/exhaustion at the workplace.       0pen and handle receptacle with care.         Prevent formation of aerosols.       Information about protection against explosions and fires:         Keep ignition sources away - Do not smoke.       100 minute for smoke.	67-56-1 Methanol	2,100 ppm
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	Handling: Precautions for safe handling Ensure good ventilation/exhaustion at the workplace. Open and handle receptacle with care. Prevent formation of aerosols. Information about protection against explosions and fires:	
Keep respiratory protective device available.	Handling: Precautions for safe handling Ensure good ventilation/exhaustion at the workplace. Open and handle receptacle with care. Prevent formation of aerosols. Information about protection against explosions and fires: Keep ignition sources away - Do not smoke. Protect against electrostatic charges.	
	Handling: Precautions for safe handling Ensure good ventilation/exhaustion at the workplace. Open and handle receptacle with care. Prevent formation of aerosols. Information about protection against explosions and fires: Keep ignition sources away - Do not smoke.	
Storage: Store in accordance with information listed on the product insert.	Handling: Precautions for safe handling Ensure good ventilation/exhaustion at the workplace. Open and handle receptacle with care. Prevent formation of aerosols. Information about protection against explosions and fires: Keep ignition sources away - Do not smoke. Protect against electrostatic charges.	
Requirements to be met by storerooms and receptacles: Store in a cool location.	<ul> <li>Handling:</li> <li>Precautions for safe handling</li> <li>Ensure good ventilation/exhaustion at the workplace.</li> <li>Open and handle receptacle with care.</li> <li>Prevent formation of aerosols.</li> <li>Information about protection against explosions and fires:</li> <li>Keep ignition sources away - Do not smoke.</li> <li>Protect against electrostatic charges.</li> <li>Keep respiratory protective device available.</li> <li>Conditions for safe storage, including any incompatibilities</li> <li>Storage: Store in accordance with information listed on the product in</li> </ul>	
	Handling:Precautions for safe handlingEnsure good ventilation/exhaustion at the workplace.Open and handle receptacle with care.Prevent formation of aerosols.Information about protection against explosions and fires:Keep ignition sources away - Do not smoke.Protect against electrostatic charges.Keep respiratory protective device available.Conditions for safe storage, including any incompatibilitiesStorage: Store in accordance with information listed on the product inRequirements to be met by storerooms and receptacles: Store in	a cool location.
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• Additional information about design of technical systems: No further data; see item 7. (Contd. on page 5)

US

Printing date 12/07/2022

Revision date 12/07/2022

## Trade name: Benzoylecgonine-d3 (CRM)

(Contd. from page 4)

Com	
	6-1 Methanol
	Long-term value: 260 mg/m³, 200 ppm
REL	Short-term value: 325 mg/m³, 250 ppm
	Long-term value: 260 mg/m³, 200 ppm
<b>T</b> 1 \ 1	Skin
ILV	Short-term value: 250 ppm Long-term value: 200 ppm
	Skin; BEI
Ingr	edients with biological limit values:
67-5	6-1 Methanol
	15 mg/L
	Medium: urine
	Time: end of shift Parameter: Methanol (background, nonspecific)
۸dd	tional information: The lists that were valid during the creation were used as basis.
Avoie Brea In ca expo	e protective clothing separately. I contact with the eyes and skin. <b>thing equipment:</b>
	se of brief exposure or low pollution use respiratory filter device. In case of intensive or long sure use respiratory protective device that is independent of circulating air. ection of hands:
	se of brief exposure or low pollution use respiratory filter device. In case of intensive or long sure use respiratory protective device that is independent of circulating air.
Due prep	The section of hands: Protective gloves Protective gloves glove material has to be impermeable and resistant to the product/ the substance/ the preparatio to missing tests no recommendation to the glove material can be given for the product/ the chemical mixture.
Due prep Sele degr	Ise of brief exposure or low pollution use respiratory filter device. In case of intensive or long sure use respiratory protective device that is independent of circulating air. Protective gloves Glove material has to be impermeable and resistant to the product/ the substance/ the preparation to missing tests no recommendation to the glove material can be given for the product/ the substance/ the produ

### Penetration time of glove material

The exact break through time has to be found out by the manufacturer of the protective gloves and has to be observed.

(Contd. on page 6)

Printing date 12/07/2022

Revision date 12/07/2022

(Contd. from page 5)

### Trade name: Benzoylecgonine-d3 (CRM)

• Eye protection:



Tightly sealed goggles

#### 9 Physical and chemical properties Information on basic physical and chemical properties General Information · Appearance: Form: Liquid Color: According to product specification · Odor: Alcohol-like · Structural Formula C16H16D3NO4 · Molecular Weight 292.3 g/mol · Odor threshold: Not determined. · Formulation A 100 µg/ml solution in methanol · pH-value: Not determined. · Change in condition Melting point/Melting range: -98 °C (-144.4 °F) **Boiling point/Boiling range:** 64.7 °C (148.5 °F) · Flash point: 11 °C (51.8 °F) · Flammability (solid, gaseous): Highly flammable. 455 °C (851 °F) · Ignition temperature: Decomposition temperature: Not determined. · Auto igniting: Product is not selfigniting. Danger of explosion: Product is not explosive. However, formation of explosive air/ vapor mixtures are possible. · Explosion limits: Lower: 5.5 Vol % 44 Vol % Upper: · Vapor pressure at 20 °C (68 °F): 128 hPa (96 mm Hg) Density at 20 °C (68 °F): 0.79 g/cm3 (6.59255 lbs/gal) Relative density Not determined. · Vapor density Not determined. · Evaporation rate Not determined. · Solubility in / Miscibility with Water: Fully miscible. · Partition coefficient (n-octanol/water): Not determined. · Viscositv: **Dynamic:** Not determined. **Kinematic:** Not determined. (Contd. on page 7)

US

Printing date 12/07/2022

Revision date 12/07/2022

Trade name: Benzoylecgonine-d3 (CRM)

	(Contd. from page 6	i)
<ul> <li>Solvent content: Organic solvents: VOC content:</li> </ul>	100.0 % 99.99 % 999.9 g/l / 8.34 lb/gal	
Solids content:	0.0 %	
· Other information	No further relevant information available.	

## **10 Stability and reactivity**

· Reactivity No further relevant information available.

- · Chemical stability
- **Thermal decomposition / conditions to be avoided:** No decomposition if used according to specifications.
- · Possibility of hazardous reactions No dangerous reactions known.
- Conditions to avoid No further relevant information available.
- · Incompatible materials: reducing agents, oxidizing agents
- · Hazardous decomposition products: carbon monoxide, carbon dioxide

## **11 Toxicological information**

· Information on toxicological effects

### · Acute toxicity:

· LD/LC50 values that are relevant for classification:			
67-56-1 Methanol			
Oral	LDLO	143 mg/kg (hmn)	
	TDLO	5 ml/kg (rat)	
	LD50	5,600 mg/kg (rat)	
Dermal	LD50	15,800 mg/kg (rabbit)	
Inhalative	LC50/4 h	64,000 mg/m³ (rat)	
	LC50	61,100 mg/m³/134 m (mouse)	
Irritation of skin	Irritation	20 mg/24h (rabbit)	
	Irritation	(rabbit)	
	Irritation	5.63 mg/kg/exempt preparation (rabbit)	
Irritation of eyes	Irritation	40 mg (rabbit)	
	Intraperitoneal TDLO	5 mg/kg (rat)	
	Intraperitoneal LD50	10,765 mg/kg (mouse)	
	Subcutaneous LD50	143 mg/kg/human (mouse)	
	Data	20 mg/24h (rabbit)	
Primary irritant effect:			

Primary irritant effect:

• on the skin: No irritant effect.

· on the eye: No irritating effect.

• Sensitization: No sensitizing effects known.

• Additional toxicological information:

The product shows the following dangers according to internally approved calculation methods for preparations:

(Contd. on page 8)

US

Printing date 12/07/2022

Revision date 12/07/2022

(Contd. from page 7)

### Trade name: Benzoylecgonine-d3 (CRM)

Toxic

· Carcinogenic categories

· IARC (International Agency for Research on Cancer)

None of the ingredients is listed.

· NTP (National Toxicology Program)

None of the ingredients is listed.

· OSHA-Ca (Occupational Safety & Health Administration)

None of the ingredients is listed.

## **12 Ecological information**

- · Toxicity
- · Aquatic toxicity: No further relevant information available.
- Persistence and degradability No further relevant information available.
- Behavior in environmental systems:
- · Bioaccumulative potential No further relevant information available.
- Mobility in soil No further relevant information available.
- · Additional ecological information:
- · General notes:

Water hazard class 2 (Self-assessment): hazardous for water

Do not allow product to reach ground water, water course or sewage system.

Danger to drinking water if even small quantities leak into the ground.

- · Results of PBT and vPvB assessment
- · **PBT:** Not applicable.
- · vPvB: Not applicable.
- Other adverse effects No further relevant information available.

## **13 Disposal considerations**

## · Waste treatment methods

· Recommendation:

Must not be disposed of together with household garbage. Do not allow product to reach sewage system.

- · Uncleaned packagings:
- Recommendation: Disposal must be made according to official regulations.
- Recommended cleansing agent: Water, if necessary with cleansing agents.

· UN-Number	
· DOT, IMDG, IATA	UN1993
UN proper shipping name	
DOT	Flammable liquids, n.o.s. (Methanol)
·IMDG	FLAMMABLE LIQUID, N.O.S. (METHANOL)
· IATA	Flammable liquid, n.o.s. (METHANOL)

Printing date 12/07/2022

Revision date 12/07/2022

Trade name: Benzoylecgonine-d3 (CRM)

Transport hazard class(es) DOT	
DOT	
RLAMARE LOUD	
Class Label	3 Flammable liquids 3
IMDG, IATA	
Class	3 Flammable liquids
Label	3
Packing group DOT, IMDG, IATA	11
Environmental hazards:	Not applicable.
Special precautions for user	Warning: Flammable liquids
Hazard identification number (Kemler code	): 33
EMS Number: Stowage Category	F-E, <u>S-E</u> B
Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code	Not applicable.
Transport/Additional information:	
DOT	
Quantity limitations	On passenger aircraft/rail: 5 L
	On cargo aircraft only: 60 L
IMDG Limited quantities (LQ)	1L
Excepted quantities (EQ)	Code: E2
	Maximum net quantity per inner packaging: 30 ml
	Maximum net quantity per outer packaging: 500 ml
IATA Remarks:	When sold in quantities of less than or equal to 1 m
	or 1 g, with an Excepted Quantity Code of
	E1, E2, E4, or E5, this item meets the De Minim
	Quantities exemption, per IATA 2.6.10. Therefore packaging does not have to be labeled a
	Dangerous Goods/Excepted Quantity.
UN "Model Regulation":	UN 1993 FLAMMABLE LIQUID, N.O.S. (METHANOL 3, II

(Contd. on page 10)

Revision date 12/07/2022

## Trade name: Benzoylecgonine-d3 (CRM)

Printing date 12/07/2022

(Contd. from page 9)

Regulatory information	
• Safety, health and environmental regulations/legislation specific for the subst No further relevant information available. • Sara	ance or mixture
Section 355 (extremely hazardous substances):	
None of the ingredients is listed.	
Section 313 (Specific toxic chemical listings):	
67-56-1 Methanol	
TSCA (Toxic Substances Control Act):	
67-56-1 Methanol	ACTIVE
· Hazardous Air Pollutants	
67-56-1 Methanol	
Proposition 65	
Chemicals known to cause cancer:	
None of the ingredients is listed.	
Chemicals known to cause reproductive toxicity for females:	
None of the ingredients is listed.	
Chemicals known to cause reproductive toxicity for males:	
None of the ingredients is listed.	
Chemicals known to cause developmental toxicity:	
67-56-1 Methanol	
Carcinogenic categories	
· EPA (Environmental Protection Agency)	
None of the ingredients is listed.	
· TLV (Threshold Limit Value)	
None of the ingredients is listed.	
NIOSH-Ca (National Institute for Occupational Safety and Health)	
None of the ingredients is listed.	

• Chemical safety assessment: A Chemical Safety Assessment has not been carried out.

## **16 Other information**

All chemicals may pose unknown hazards and should be used with caution. This SDS applies only to the material as packaged. If this product is combined with other materials, deteriorates, or becomes contaminated, it may pose hazards not mentioned in this SDS. Cayman Chemical Company assumes no responsibility for incidental or consequential damages, including lost profits, arising from the use of these data. It shall be the user's responsibility to develop proper methods of handling and personal protection based on the actual conditions of use. While this SDS is based on technical data judged to be reliable, Cayman Chemical Company assumes no responsibility for the completeness or accuracy of the information contained herein.

- · Department issuing SDS: Environment protection department.
- · Contact: -
- Date of preparation / last revision 12/07/2022
- **Abbreviations and acronyms:** IMDG: International Maritime Code for Dangerous Goods DOT: US Department of Transportation

Printing date 12/07/2022

Revision date 12/07/2022

## Trade name: Benzoylecgonine-d3 (CRM)

	(Contd. from page 10)
IATA: International Air Transport Association	13 1
EINECS: European Inventory of Existing Commercial Chemical Substances	
ELINCS: European List of Notified Chemical Substances	
CAS: Chemical Abstracts Service (division of the American Chemical Society)	
NFPA: National Fire Protection Association (USA)	
HMIS: Hazardous Materials Identification System (USA)	
VOC: Volatile Organic Compounds (USA, EU)	
LC50: Lethal concentration, 50 percent	
LD50: Lethal dose, 50 percent	
PBT: Persistent, Bioaccumulative and Toxic	
vPvB: very Persistent and very Bioaccumulative	
NIOSH: National Institute for Occupational Safety	
OSHA: Occupational Safety & Health	
TLV: Threshold Limit Value	
PEL: Permissible Exposure Limit	
REL: Recommended Exposure Limit	
BEI: Biological Exposure Limit	
Flammable Liquids 2: Flammable liquids – Category 2	
Acute Toxicity - Oral 3: Acute toxicity - Category 3	
Specific Target Organ Toxicity - Single Exposure 1: Specific target organ toxicity (single exposure) - Catego	jory 1
	Us