

# MATERIAL SAFETY DATA SHEET

## 5(S),6(R)-7-trihydroxymethyl Heptanoate

Cayman Chemical Company  
1180 E. Ellsworth Rd.  
Ann Arbor, MI 48108

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### 1. Product and Company Identification

**Product Code:** 10005032  
**Product Name:** 5(S),6(R)-7-trihydroxymethyl Heptanoate  
**Manufacturer Information**  
**Company Name:** Cayman Chemical Company  
**Emergency Contact:** Cayman Chemical Company (800)364-9897  
**Information:** Cayman Chemical Company (734)971-3335  
**Chemical Family:** Agonists & Antagonists  
**Synonyms:** 5S,6R-trihydroxy-7-heptanoic acid, methyl ester; BML-111;

### 2. Composition/Information on Ingredients

Hazardous Components (Chemical Name)	CAS #	Concentration	OSHA TWA	ACGIH TWA	Other Limits
1. 5(S),6(R)-7-trihydroxymethyl Heptanoate	NA	1.0 %	No data.	No data.	No data.
2. Methanol	67-56-1	99.0 %	8H TWA:200 ppm (260 mg/m3)	TWA 200 ppm (262 mg/m3 skin)	No data.

  

Hazardous Components (Chemical Name)	RTECS #	OSHA STEL	OSHA CEIL	ACGIH STEL	ACGIH CEIL
1. 5(S),6(R)-7-trihydroxymethyl Heptanoate	NA	No data.	No data.	No data.	No data.
2. Methanol	PC1400000	325 mg/m3 skin	No data.	250 ppm (328 mg/m3 skin)	No data.

### 3. Hazards Identification

**Emergency Overview:** No data available.

**Route(s) of Entry:** Inhalation? Yes Skin? Yes Eyes? Yes Ingestion? Yes Other: Injection

**Potential Health Effects (Acute and Chronic):** The hazards identified with this product are those associated with the solvent(s).  
 Cannot be made nonpoisonous.  
 Extremely hazardous in case of ingestion.  
 Irritating to eyes, respiratory system and skin.  
 Material is irritating to the mucous membranes and upper respiratory tract.  
 May be fatal if swallowed or inhaled.  
 May be harmful by inhalation, ingestion, or skin absorption.  
 Please refer to Section 11 for behavioral, developmental, embryo, fetal, or paternal chronic effects.  
 Poison.  
 Repeated exposure may cause skin dryness or cracking.  
 The toxicological properties of this compound have not been fully evaluated.  
 Toxic.  
 Toxic if inhaled, absorbed through skin, or swallowed.

**LD 50 / LC 50:** Please refer to Section 11

**Signs and Symptoms Of Exposure:** Eye inflammation is characterized by redness, watering, and itching.  
 Ingestion can cause: Nausea, headache, vomiting, gastrointestinal disturbances, dizziness, weakness, confusion, drowsiness and unconsciousness.  
 May cause convulsions.  
 Methyl alcohol may be fatal or cause blindness if swallowed.  
 Overexposure can cause: headache, drowsiness, nausea, vomiting, blurred vision, blindness, coma, and death. A person may get better then worsen up to 30 hours later.  
 Skin inflammation is characterized by itching, scaling, reddening, or, occasionally, blistering.

**Medical Conditions Generally Aggravated By Exposure:** Persons with pre-existing skin disorders or eye problems or impaired liver or kidney function may be more susceptible to the effects of the substance.

### 4. First Aid Measures

**Emergency and First Aid Procedures:** If inhaled remove to fresh air. If not breathing, give artificial respiration or give oxygen by trained personnel. Get immediate medical attention.  
Do not give direct mouth-to-mouth if victim ingested or inhaled this substance; induce artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device.  
If swallowed, wash out mouth with water provided person is conscious. Never give anything by mouth to an unconscious person. Get medical attention. Do NOT induce vomiting unless directed to do so by medical personnel.  
In case of contact with eyes, hold eyelids apart and flush eyes with plenty of water. After initial flushings, remove any contact lenses and continue flushing for at least 20 minutes. Have eyes examined and tested by medical personnel.  
In case of skin contact, immediately wash skin with soap and plenty of water. Remove contaminated clothing. Get medical attention if symptoms occur. Wash clothing before reuse.

### 5. Fire Fighting Measures

**Flash Pt:** 12.00 C Method Used: CC  
**Explosive Limits:** LEL: 6% at 25.0 C UEL: 36% at 25.0 C  
**Autoignition Pt:** 464.00 C  
**Fire Fighting Instructions:** As in any fire, wear self-contained breathing apparatus pressure-demand (MSHA/NIOSH approved or equivalent), and full protective gear to prevent contact with skin and eyes.  
Note: Flammable as diluted in methanol.  
**Flammable Properties and Hazards:** Can release vapors that form explosive mixtures at temperatures at or above the flashpoint. Container explosion may occur under fire conditions.  
Emits toxic fumes under fire conditions.  
Flammable Liquid.  
Sensitive to static discharge.  
Vapors can travel to a source of ignition and flash back.  
**Extinguishing Media:** Use alcohol-resistant foam, carbon dioxide, water, or dry chemical spray when fighting fires involving this material.  
Use water spray to cool fire-exposed containers.  
**Unsuitable Extinguishing Media:** No data available.

### 6. Accidental Release Measures

**Steps To Be Taken In Case Material Is Released Or Spilled:** Wear a NIOSH/MSHA approved self-contained breathing apparatus and appropriate personal protection (rubber boots, safety goggles, and heavy rubber gloves).  
Absorb spill with inert material (e.g. dry sand or earth), then place in a chemical waste container.  
After removal, ventilate contaminated area and flush thoroughly with water.  
Avoid release into the environment - very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

### 7. Handling and Storage

**Hazard Label Information:** Avoid contact with skin and eyes. Do not reuse this container. Use with adequate ventilation.  
Wash thoroughly after handling.  
**Precautions To Be Taken in Handling:** Avoid breathing (dust, vapor, mist, gas).  
Avoid contact with eyes, skin, and clothing.  
Avoid prolonged or repeated exposure.  
Do not reuse this container.  
Keep away from sources of ignition.  
Use with adequate ventilation.  
Wash thoroughly after handling.  
**Precautions To Be Taken in Storing:** Store at correct temperature.

### 8. Exposure Controls/Personal Protection

<b>Protective Equipment Summary - Hazard Label Information:</b>	Eye wash station in work area    Lab coat    Latex disposable gloves    Safety glasses    Safety shower in work area    Vent Hood
<b>Respiratory Equipment (Specify Type):</b>	Government approved respirator as conditions warrant.
<b>Eye Protection:</b>	Safety glasses
<b>Protective Gloves:</b>	Latex disposable gloves
<b>Other Protective Clothing:</b>	Lab coat
<b>Engineering Controls (Ventilation etc.):</b>	Use process enclosures, local exhaust ventilation, or other engineering controls to control airborne levels below recommended exposure limits.
<b>Work/Hygienic/Maintenance Practices:</b>	Do not take internally. Facilities storing or utilizing this material should be equipped with an eyewash facility and a safety shower. Wash thoroughly after handling.

### 9. Physical and Chemical Properties

<b>Physical States:</b>	<input type="checkbox"/> Gas <input checked="" type="checkbox"/> Liquid <input type="checkbox"/> Solid
<b>Melting Point:</b>	No data.
<b>Boiling Point:</b>	No data.
<b>Autoignition Pt:</b>	464.00 C
<b>Flash Pt:</b>	12.00 C    Method: CC
<b>Explosive Limits:</b>	LEL: 6%    at 25.0 C    UEL: 36%    at 25.0 C
<b>Specific Gravity (Water = 1):</b>	No data.
<b>Vapor Pressure (vs. Air or mm Hg):</b>	97 MM_HG    at 20.0 C
<b>Vapor Density (vs. Air = 1):</b>	No data.
<b>Evaporation Rate (vs Butyl Acetate=1):</b>	No data.
<b>Solubility in Water:</b>	10 mg/ml*    at 25.0 C
<b>Other Solubility Notes:</b>	*PBS pH 7.2, also sol. in DMF, DMSO, & EtOH, see product insert.
<b>Percent Volatile:</b>	No data.
<b>Corrosion Rate:</b>	No data.
<b>Formula:</b>	C8H16O5
<b>Molecular Weight:</b>	192.20
<b>pH:</b>	No data.
<b>Appearance and Odor:</b>	A clear, colorless solution

### 10. Stability and Reactivity

<b>Stability:</b>	Unstable <input type="checkbox"/> Stable <input checked="" type="checkbox"/>
<b>Conditions To Avoid - Instability:</b>	may react with metallic aluminum and generate hydrogen gas protect from heat protect from ignition sources
<b>Incompatibility - Materials To Avoid:</b>	acids acid anhydrides acid chlorides alkali metals metals nitrates oxidizing agents perchlorates reducing agents sulfuric acid
<b>Hazardous Decomposition Or Byproducts:</b>	carbon dioxide carbon monoxide formaldehyde

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**Hazardous Polymerization:** Will occur [ ] Will not occur [ X ]  
**Conditions To Avoid - Hazardous Polymerization:** No data available.

### 11. Toxicological Information

**Toxicological Information:** The toxicological effects of this compound have not been thoroughly studied.

#### Methanol - Toxicity Data:

Oral LDLO (man):6422 mg/kg

Oral LDLO (human):143 mg/kg

Oral LD50 (rat):5628 mg/kg

Skin LD50 (rabbit): 15800 mg/kg

Subcutaneous LD50 (mouse):9800 mg/kg

Inhalation LD50 (rat):64,000 ppm/4H

Intraperitoneal LD50 (rat):7529 mg/kg

Intraperitoneal LD50 (mouse):10765 mg/kg

Intraperitoneal LD50 (rabbit):1826 mg/kg

#### Methanol - Irritation Data:

Skin (rabbit): 20 mg 24H moderate effect

Eyes (rabbit): 100 mg 24H moderate effect

**Chronic Toxicological Effects:** Methanol - Investigated as a teratogen, mutagen, and reproductive effector.

#### Methanol Chronic Exposure:

Behavioral: Muscle weakness; Ataxia; Coma

Effects on embryo or fetus (fetal death)

Effects on embryo or fetus (fetotoxicity)

Effects on fertility (litter size)

Effects on fertility (pre-implantation mortality)

Effects on fertility (post-implantation mortality)

Effects on newborn (Behavioral)

Effects on newborn (Biochemical and metabolic)

Paternal effects (spermatogenesis)

Paternal effects (testes, epidymis, sperm duct)

Specific developmental abnormalities (cardiovascular (circulatory) system)

Specific developmental abnormalities (central nervous system)

Specific developmental abnormalities (craniofacial, including nose and tongue)

Specific developmental abnormalities (eye, ear)

Specific developmental abnormalities (endocrine system)

Specific developmental abnormalities (musculoskeletal system)

Specific developmental abnormalities (urogenital system)

Only select Registry of Toxic Effects of Chemical Substances (RTECS) data is presented here.

See actual entry in RTECS for complete information.

Methanol RTECS Number: PC1400000

**Carcinogenicity/Other Information:** No data available.

**Carcinogenicity:** NTP? No IARC Monographs? No OSHA Regulated? No

### 12. Ecological Information

**Ecological Information:** Avoid release into the environment - very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.  
Runoff from fire control or dilution water may cause pollution.

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**13. Disposal Considerations**

**Waste Disposal Method:** Dispose in accordance with local, state and federal regulations.

**14. Transport Information**

**LAND TRANSPORT (US DOT)**

**DOT Proper Shipping Name** Methanol  
**DOT Hazard Class:** 3  
**DOT Hazard Label:** FLAMMABLE LIQUID, TOXIC  
**UN/NA Number:** 1230  
**Packing Group:** II

**Additional Transport Information:** Transport in accordance with local, state, and federal regulations.

**15. Regulatory Information**

**US EPA SARA Title III**

Hazardous Components (Chemical Name)	CAS #	Sec.302 (EHS)	Sec.304 RQ	Sec.313 (TRI)	Sec.110
1. 5(S),6(R)-7-trihydroxymethyl Heptanoate	NA	No	No	No	No
2. Methanol	67-56-1	No	Yes 5000 LB	Yes	No

**US EPA CAA, CWA, TSCA**

Hazardous Components (Chemical Name)	CAS #	EPA CAA	EPA CWA NPDES	EPA TSCA	CA PROP 65
1. 5(S),6(R)-7-trihydroxymethyl Heptanoate	NA	No	No	No	No
2. Methanol	67-56-1	HAP	No	Inventory	No

**16. Other Information**

**Company Policy or Disclaimer**

For research use only, not for human or veterinary clinical use.

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