

## O-4-METHYLCOUMARINYL-N-[3-(TRIETHOXSILYL)PROPYL]CARBAMATE

Safety Data Sheet SIM6502.0

Date of issue: 10/06/2015 Version: 1.1

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

#### 1.1. Product identifier

Product form : Substance  
 Physical state : Solid  
 Substance name : O-4-METHYLCOUMARINYL-N-[3-(TRIETHOXSILYL)PROPYL]CARBAMATE  
 Product code : SIM6502.0  
 Formula : C<sub>20</sub>H<sub>29</sub>NO<sub>7</sub>Si  
 Synonyms : O-4-METHYLCOUMARINYL-N-[3-(TRIETHOXSILYL)PROPYL]URETHANE  
 Chemical family : ORGANOETHOXSILANE

#### 1.2. Relevant identified uses of the substance or mixture and uses advised against

Use of the substance/mixture : Chemical intermediate  
 For research use only

#### 1.3. Details of the supplier of the safety data sheet

##### GELEST, INC.

11 East Steel Road  
 Morrisville, PA 19067

##### USA

T 215-547-1015 - F 215-547-2484 - (M-F): 8:00 AM - 5:30 PM EST

[info@gelest.com](mailto:info@gelest.com) - [www.gelest.com](http://www.gelest.com)

#### 1.4. Emergency telephone number

Emergency number : CHEMTREC: 1-800-424-9300 (USA); +1 703-527-3887 (International)

### SECTION 2: Hazards identification

#### 2.1. Classification of the substance or mixture

##### GHS-US classification

Skin Irrit. 2 H315  
 Eye Irrit. 2A H319  
 STOT SE 3 H335

Full text of H-phrases: see section 16

#### 2.2. Label elements

##### GHS-US labeling

Hazard pictograms (GHS-US) :



GHS07

Signal word (GHS-US) : Warning

Hazard statements (GHS-US) : H315 - Causes skin irritation  
 H319 - Causes serious eye irritation  
 H335 - May cause respiratory irritation

Precautionary statements (GHS-US) : P280 - Wear protective gloves/protective clothing/eye protection/face protection  
 P261 - Avoid breathing dust  
 P264 - Wash hands thoroughly after handling  
 P271 - Use only outdoors or in a well-ventilated area  
 P304+P340 - If inhaled: Remove person to fresh air and keep comfortable for breathing  
 P302+P352 - If on skin: Wash with plenty of soap and water  
 P332+P313 - If skin irritation occurs: Get medical advice/attention  
 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  
 P312 - Call a doctor if you feel unwell  
 P362 - Take off contaminated clothing and wash it before reuse  
 P403+P233 - Store in a well-ventilated place. Keep container tightly closed  
 P405 - Store locked up  
 P501 - Dispose of contents/container to licensed waste disposal facility.  
 P321 - Specific treatment (see first aid instructions on this label)

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### 2.3. Other hazards

Other hazards not contributing to the classification : Additional ethanol may be formed by reaction with moisture and water. The hydrolysis product of this compound is ethanol. Overexposure to ethanol by skin absorption, inhalation or ingestion may have a narcotic effect (headache, nausea, drowsiness). Ethanol is metabolized to acetaldehyde and acetic acid which in large quantities result in metabolic acidosis, CNS depression and death due to respiratory arrest. The US OSHA PEL (TWA) for ethanol is 1000 ppm. This product contains ethanol which is classified as a carcinogen by IARC in alcoholic beverages.

### 2.4. Unknown acute toxicity (GHS US)

No data available

## SECTION 3: Composition/Information on ingredients

### 3.1. Substance

Substance type : Mono-constituent  
Name : O-4-METHYLCOUMARINYL-N-[3-(TRIETHOXSILYL)PROPYL]CARBAMATE  
CAS No : 129119-78-4

Name	Product identifier	%	GHS-US classification
O-4-Methylcoumarinyl-N-[3-(triethoxysilyl)propyl]carbamate	(CAS No) 129119-78-4	95 - 100	Skin Irrit. 2, H315 Eye Irrit. 2A, H319 STOT SE 3, H335

### 3.2. Mixture

Not applicable

## SECTION 4: First aid measures

### 4.1. Description of first aid measures

First-aid measures general : Remove contaminated clothing and shoes. In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible). If possible show this sheet; if not available show packaging or label. IF exposed or concerned: Get medical advice/attention.

First-aid measures after inhalation : Remove victim to fresh air and keep at rest in a position comfortable for breathing. If you feel unwell, seek medical advice.

First-aid measures after skin contact : Wash with plenty of soap and water. Get medical advice/attention.

First-aid measures after eye contact : Immediately flush eyes thoroughly with water for at least 15 minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Get medical advice/attention.

First-aid measures after ingestion : Never give anything by mouth to an unconscious person. Get medical advice/attention.

### 4.2. Most important symptoms and effects, both acute and delayed

Symptoms/injuries after inhalation : May cause respiratory irritation.

Symptoms/injuries after skin contact : Causes skin irritation.

Symptoms/injuries after eye contact : Causes serious eye irritation.

Symptoms/injuries after ingestion : May be harmful if swallowed.

Chronic symptoms : On contact with water this compound liberates ethanol which is known to have a chronic effect on the central nervous system.

### 4.3. Indication of any immediate medical attention and special treatment needed

NOTE TO PHYSICIAN: This product reacts with water in the acid contents of the stomach to form ethanol.

## SECTION 5: Firefighting measures

### 5.1. Extinguishing media

Suitable extinguishing media : Water spray. Foam. Carbon dioxide. Dry chemical.

Unsuitable extinguishing media : Do not use straight streams.

### 5.2. Special hazards arising from the substance or mixture

Fire hazard : Irritating fumes and organic acid vapors may develop when material is exposed to elevated temperatures or open flame.

### 5.3. Advice for firefighters

Firefighting instructions : Use water spray to cool exposed surfaces. Exercise caution when fighting any chemical fire.

Protection during firefighting : Do not enter fire area without proper protective equipment, including respiratory protection. Avoid contact with skin and eyes. Do not breathe dust.

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### SECTION 6: Accidental release measures

#### 6.1. Personal precautions, protective equipment and emergency procedures

##### 6.1.1. For non-emergency personnel

Protective equipment : Wear protective equipment as described in Section 8.

Emergency procedures : Evacuate unnecessary personnel.

##### 6.1.2. For emergency responders

Protective equipment : Do not attempt to take action without suitable protective equipment. Equip cleanup crew with proper protection. For further information refer to section 8: "Exposure controls/personal protection".

#### 6.2. Environmental precautions

Prevent entry to sewers and public waters. Notify authorities if product enters sewers or public waters.

#### 6.3. Methods and material for containment and cleaning up

For containment : Contain any spills with dikes or absorbents to prevent migration and entry into sewers or streams.

Methods for cleaning up : Clean up any spills as soon as possible, using an absorbent material to collect it. Sweep or shovel spills into appropriate container for disposal.

#### 6.4. Reference to other sections

See Heading 8. Exposure controls and personal protection.

### SECTION 7: Handling and storage

#### 7.1. Precautions for safe handling

Precautions for safe handling : Avoid contact with skin and eyes. Avoid dust formation. Do not breathe dust. Use only outdoors or in a well-ventilated area.

Hygiene measures : Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work. Wash contaminated clothing before reuse.

#### 7.2. Conditions for safe storage, including any incompatibilities

Storage conditions : Keep container tightly closed. Store locked up.

Incompatible materials : Acids. Alcohols. Oxidizing agent. Peroxides. Moisture. Water.

Storage area : Store in a well-ventilated place. Store away from heat.

#### 7.3. Specific end use(s)

No additional information available

### SECTION 8: Exposure controls/personal protection

#### 8.1. Control parameters

No additional information available

#### 8.2. Exposure controls

Appropriate engineering controls : Provide local exhaust or general room ventilation.

Personal protective equipment : Avoid all unnecessary exposure. Emergency eye wash fountains and safety showers should be available in the immediate vicinity of any potential exposure.

Hand protection : Neoprene or nitrile rubber gloves.

Eye protection : Chemical goggles. Contact lenses should not be worn.

Skin and body protection : Wear suitable protective clothing.

Respiratory protection : Where exposure through inhalation may occur from use, respiratory protection equipment is recommended. NIOSH-certified dust and mist (orange cartridge) respirator.

### SECTION 9: Physical and chemical properties

#### 9.1. Information on basic physical and chemical properties

Physical state : Solid

Appearance : Solid.

Molecular mass : 423.54 g/mol

Color : Off-white to amber.

Odor : No data available

Odor threshold : No data available

Refractive index : No data available

pH : No data available

Relative evaporation rate (butyl acetate=1) : No data available

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Melting point	: 88 - 90 °C
Freezing point	: No data available
Boiling point	: > 100 °C @ 0.1 mm Hg
Flash point	: > 110 °C
Auto-ignition temperature	: No data available
Decomposition temperature	: No data available
Flammability (solid, gas)	: No data available
Vapor pressure	: < 1 mm Hg @ 25°C
Relative vapor density at 20 °C	: No data available
Relative density	: > 1
VOC content	: < 5 %
Solubility	: Reacts with water. Organic solvent:Soluble: THF
Log Pow	: No data available
Log Kow	: No data available
Viscosity, kinematic	: No data available
Viscosity, dynamic	: No data available
Explosive properties	: No data available
Oxidizing properties	: No data available
Explosion limits	: No data available

### 9.2. Other information

No additional information available

## SECTION 10: Stability and reactivity

### 10.1. Reactivity

No additional information available

### 10.2. Chemical stability

Stable when stored in sealed containers.

### 10.3. Possibility of hazardous reactions

Reacts with water and moisture in air, liberating ethanol.

### 10.4. Conditions to avoid

Heat. Open flame. Sparks.

### 10.5. Incompatible materials

Acids. Alcohols. Oxidizing agent. Peroxides. Moisture. Water.

### 10.6. Hazardous decomposition products

Ethanol. Organic acid vapors.

## SECTION 11: Toxicological information

### 11.1. Information on toxicological effects

Acute toxicity	: Not classified
Skin corrosion/irritation	: Causes skin irritation.
Serious eye damage/irritation	: Causes serious eye irritation.
Respiratory or skin sensitization	: Not classified
Germ cell mutagenicity	: Not classified
Carcinogenicity	: Not classified
Reproductive toxicity	: Not classified
Specific target organ toxicity (single exposure)	: May cause respiratory irritation.
Specific target organ toxicity (repeated exposure)	: Not classified
Aspiration hazard	: Not classified
Potential Adverse human health effects and symptoms	: This compound liberates ethanol on contact with moisture. Material generates ethanol on contact with water or moisture in skin, eyes and mucous membranes and has an irritating, dehydrating effect on overexposed tissue.
Symptoms/injuries after inhalation	: May cause respiratory irritation.
Symptoms/injuries after skin contact	: Causes skin irritation.

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Symptoms/injuries after eye contact	: Causes serious eye irritation.
Symptoms/injuries after ingestion	: May be harmful if swallowed.
Chronic symptoms	: On contact with water this compound liberates ethanol which is known to have a chronic effect on the central nervous system.
Reason for classification	: Expert judgment

### SECTION 12: Ecological information

#### 12.1. Toxicity

No additional information available

#### 12.2. Persistence and degradability

No additional information available

#### 12.3. Bioaccumulative potential

No additional information available

#### 12.4. Mobility in soil

No additional information available

#### 12.5. Other adverse effects

Other adverse effects	: This substance may be hazardous to the environment.
Effect on ozone layer	: No additional information available
Effect on the global warming	: No known ecological damage caused by this product.

### SECTION 13: Disposal considerations

#### 13.1. Waste treatment methods

Sewage disposal recommendations	: Do not dispose of waste into sewer.
Waste disposal recommendations	: Dispose in a safe manner in accordance with local/national regulations. Dispose of contents/container to licensed waste disposal facility.
Ecology - waste materials	: Avoid release to the environment.

### SECTION 14: Transport information

#### 14.1. UN number

Not regulated for transport.

#### 14.2. UN proper shipping name

Not applicable

#### 14.3. Additional information

Other information : No supplementary information available.

#### Transport by sea

No additional information available

#### Air transport

No additional information available

### SECTION 15: Regulatory information

#### 15.1. US Federal regulations

##### O-4-METHYLCOUMARINYL-N-[3-(TRIETHOXSILYL)PROPYL]CARBAMATE (129119-78-4)

TSCA Exemption/Exclusion

CAUTION: This material is supplied for research and development purposes subject to the R&D exemption under TSCA, 40 CFR 720.36, and must meet the requirements of the exemption, including supervision by a "technically qualified individual" as defined by 40 CFR 720.3(ee). The use of this material for "commercial purposes" as defined by 40 CFR 720.3(r) is not permitted in the United States.

##### O-4-Methylcoumarinyl-N-[3-(triethoxysilyl)propyl]carbamate (129119-78-4)

Not listed on the United States TSCA (Toxic Substances Control Act) inventory

#### 15.2. International regulations

No additional information available

#### 15.3. US State regulations

##### O-4-METHYLCOUMARINYL-N-[3-(TRIETHOXSILYL)PROPYL]CARBAMATE(129119-78-4)

U.S. - California - Proposition 65 - Carcinogens List | No

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O-4-METHYLCOUMARINYL-N-[3-(TRIETHOXSILYL)PROPYL]CARBAMATE(129119-78-4)				
U.S. - California - Proposition 65 - Developmental Toxicity		No		
U.S. - California - Proposition 65 - Reproductive Toxicity - Female		No		
U.S. - California - Proposition 65 - Reproductive Toxicity - Male		No		
O-4-Methylcoumarinyl-N-[3-(triethoxysilyl)propyl]carbamate (129119-78-4)				
U.S. - California - Proposition 65 - Carcinogens List	U.S. - California - Proposition 65 - Developmental Toxicity	U.S. - California - Proposition 65 - Reproductive Toxicity - Female	U.S. - California - Proposition 65 - Reproductive Toxicity - Male	Non-significant risk level (NSRL)
No	No	No	No	

### SECTION 16: Other information

#### Abbreviations and acronyms

: Abbreviations: ND: Not Determined, No Data; NA: Not Applicable; LD: Lethal Dose; LC: Lethal Concentration; ATE: Acute Toxicity Estimates; H: hour; °: °C unless otherwise stated; mm: millimeters Hg, torr; PEL: permissible exposure level; TWA: time weighted average; TLV: threshold limit value; TG: Test Guideline; NIOSH: National Institute for Occupational Safety and Health; IARC: International Agency for Research on Cancer; NTP: National Toxicology Program; HMIS: Hazardous Material Information System; CAS No.: Chemical Abstract Service Registration Number; EC No.: European Commission Registration Number; EC Index No.: European Commission Index Number; OECD: The Organisation for Economic Co-operation and Development.

#### Full text of H-phrases::

Eye Irrit. 2A	Serious eye damage/eye irritation Category 2A
Skin Irrit. 2	Skin corrosion/irritation Category 2
STOT SE 3	Specific target organ toxicity (single exposure) Category 3
H315	Causes skin irritation
H319	Causes serious eye irritation
H335	May cause respiratory irritation

#### HMIS III Rating

Health : 2 Moderate Hazard - Temporary or minor injury may occur  
Flammability : 1 Slight Hazard  
Physical : 1 Slight Hazard

Prepared by safety and environmental affairs.

Date of issue: 10/06/2015 Version: 1.1

SDS US (GHS HazCom 2012) - Custom

According to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

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