



# ETHYL ACETOACETATE (3-13C, 99%)

## Safety Data Sheet

according to Regulation (EC) No. 1907/2006 (REACH) with its amendment Regulation (EU) 2015/830 and according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

Date of issue: 14/01/2011  
CLM-681

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Version: 3.0

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

#### 1.1. Product identifier

Product form : Substance  
Substance name : ETHYL ACETOACETATE (3-13C, 99%)  
EC No : 205-516-1 (Unlabeled)  
CAS No : 144634-49-1  
Product code : CLM-681  
Formula :  $\text{CH}_3^*\text{COCH}_2\text{COOCH}_2\text{CH}_3$   
Synonyms : Acetoacetic ester

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

##### 1.2.1. Relevant identified uses

Main use category : Professional use  
Industrial/Professional use spec : For professional use only

##### 1.2.2. Uses advised against

No additional information available

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

Cambridge Isotope Laboratories, Inc.  
50 Frontage Road  
Andover, MA 01810  
USA

USA: 1-800-322-1174 Int: 1-978-749-8000  
[cilsales@isotope.com](mailto:cilsales@isotope.com) [www.isotope.com](http://www.isotope.com)

#### Emergency telephone number

Emergency numbers:

Chemtrec: 1-800-424-9300 (24 hours)  
International: 1-703-741-5970 (24 hours)

### SECTION 2: Hazards identification

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

##### Classification according to Regulation (EC) No. 1272/2008 [CLP]

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

Full text of hazard classes and H-statements : see section 16

##### Classification according to Directive 67/548/EEC [DSD] or 1999/45/EC [DPD]

Xi; R36/37/38

Full text of R-phrases: see section 16

##### GHS-US classification

Flam. Liq. 4 H227  
Skin Irrit. 2 H315  
Eye Irrit. 2A H319  
STOT SE 3 H335

Full text of H statements : see section 16

##### Adverse physicochemical, human health and environmental effects

No additional information available

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### 2.2. Label elements

#### Labelling according to Regulation (EC) No. 1272/2008 [CLP]

Hazard pictograms (CLP) :



GHS07

Signal word (CLP) :

Warning

Hazard statements (CLP) :

H315 - Causes skin irritation  
H319 - Causes serious eye irritation  
H335 - May cause respiratory irritation

Precautionary statements (CLP) :

P261 - Avoid breathing mist, dust, fume, gas, spray, vapours  
P264 - Wash hands, forearms and face thoroughly after handling  
P271 - Use only outdoors or in a well-ventilated area  
P280 - Wear eye protection, face protection, protective clothing, protective gloves  
P302+P352 - IF ON SKIN: Wash with plenty of soap and water  
P304+P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing  
P305+P351+P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing  
P312 - Call a doctor if you feel unwell

#### GHS-US labelling

Hazard pictograms (GHS-US) :



GHS07

Signal word (GHS-US) :

Warning

Hazard statements (GHS-US) :

H227 - Combustible liquid  
H315 - Causes skin irritation  
H319 - Causes serious eye irritation  
H335 - May cause respiratory irritation

Precautionary statements (GHS-US) :

P210 - Keep away from heat, hot surfaces, open flames, sparks. - No smoking  
P261 - Avoid breathing dust, mist, fume, gas, spray, vapours  
P264 - Wash hands, forearms and face thoroughly after handling  
P271 - Use only outdoors or in a well-ventilated area  
P280 - Wear eye protection, face protection, protective clothing, protective gloves  
P302+P352 - If on skin: Wash with plenty of water  
P304+P340 - If inhaled: Remove person to fresh air and keep comfortable for breathing  
P305+P351+P338 - If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing  
P312 - Call a doctor if you feel unwell  
P321 - Specific treatment (see Hazardous component(s) for labelling on this label)  
P332+P313 - If skin irritation occurs: Get medical advice/attention  
P337+P313 - If eye irritation persists: Get medical advice/attention  
P362 - Take off contaminated clothing and wash before reuse  
P370+P378 - In case of fire: Use alcohol resistant foam, carbon dioxide (CO<sub>2</sub>), dry extinguishing powder 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 hazardous or special waste collection point, in accordance with local, regional, national and/or international regulation

### 2.3. Other hazards

No additional information available

## SECTION 3: Composition/information on ingredients

### 3.1. Substances

| Name                            | Product identifier                                    | %   | Classification according to Directive 67/548/EEC |
|---------------------------------|---|-----|--|
| ETHYL ACETOACETATE (3-13C, 99%) | (CAS No) 144634-49-1<br>(EC No) 205-516-1 (Unlabeled) | 100 | Xi; R36/37/38                                    |

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| Name                            | Product identifier                                    | %   | Classification according to Regulation (EC) No. 1272/2008 [CLP] |
|---------------------------------|---|-----|---|
| ETHYL ACETOACETATE (3-13C, 99%) | (CAS No) 144634-49-1<br>(EC No) 205-516-1 (Unlabeled) | 100 | Skin Irrit. 2, H315<br>Eye Irrit. 2, H319<br>STOT SE 3, H335    |

Full text of R- and H-statements: see section 16

| Name  | Product identifier   | %   | GHS-US classification   |
|---|----------------------|-----|---|
| ETHYL ACETOACETATE (3-13C, 99%)<br>(Main constituent) | (CAS No) 144634-49-1 | 100 | Flam. Liq. 4, H227<br>Skin Irrit. 2, H315<br>Eye Irrit. 2A, H319<br>STOT SE 3, H335 |

Full text of H-statements: see section 16

### 3.2. Mixtures

Not applicable

## SECTION 4: First aid measures

### 4.1. Description of first aid measures

|                                       |  |
|---------------------------------------|--|
| First-aid measures general            | : If you feel unwell, seek medical advice (show the label where possible). Evacuate danger area.   |
| First-aid measures after inhalation   | : When symptoms occur: go into open air and ventilate suspected area. If not breathing, give artificial respiration. Get medical advice/attention. Remove victim to fresh air and keep at rest in a position comfortable for breathing. Call a POISON CENTER or doctor/physician if you feel unwell.   |
| First-aid measures after skin contact | : Wash with plenty of soap and water. Get immediate medical advice/attention. Wash with plenty of soap and water. Wash contaminated clothing before reuse. If skin irritation occurs: Gently wash with plenty of soap and water, Get immediate medical advice/attention. Get medical advice/attention. Specific treatment (see Hazard pictograms (CLP) on this label). |
| First-aid measures after eye contact  | : Rinse cautiously with water for several minutes.   |
| First-aid measures after ingestion    | : Never give anything by mouth to an unconscious person. Rinse mouth out with water. Get medical advice/attention.   |

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

|                                      |  |
|--------------------------------------|--|
| Symptoms/injuries after inhalation   | : May be harmful if inhaled. 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.                                 |

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

No additional information available

## SECTION 5: Fire-fighting measures

### 5.1. Extinguishing media

Suitable extinguishing media : Water spray, dry chemical powder, alcohol-resistant foam, carbon dioxide (CO<sub>2</sub>).

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

No additional information available

### 5.3. Advice for firefighters

|                                |   |
|--------------------------------|---|
| Firefighting instructions      | : Fight fire with normal precautions from a reasonable distance. Wear a self contained breathing apparatus. Do not enter fire area without proper protective equipment, including respiratory protection. |
| Protection during firefighting | : Do not enter fire area without proper protective equipment, including respiratory protection. Wear recommended personal protective equipment.   |
| Other information              | : Use water spray to cool exposed surfaces.   |

## SECTION 6: Accidental release measures

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

#### 6.1.1. For non-emergency personnel

Emergency procedures : Use personal protective equipment, and ensure adequate ventilation. Avoid breathing vapors, mist, gas. Remove ignition sources, and move personnel to safe area. Vapors accumulate especially in low areas to form explosive concentrations.

#### 6.1.2. For emergency responders

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

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### 6.2. Environmental precautions

Prevent entry to sewers and public waters. Do not allow to enter drains or water courses. Avoid release to the environment.

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

- For containment : Collect spillage. Clean up any spills as soon as possible, using an absorbent material to collect it. Small quantities of liquid spill: take up in non-combustible absorbent material and shovel into container for disposal. For large spills, confine the spill in a dike and charge it with wet sand or earth for subsequent safe disposal.
- Methods for cleaning up : This material and its container must be disposed of in a safe way, and as per local legislation.

### 6.4. Reference to other sections

No additional information available

## SECTION 7: Handling and storage

### 7.1. Precautions for safe handling

- Additional hazards when processed : Avoid all eye and skin contact and do not breathe vapour and mist. Take precautionary measures against static discharges. Do not breathe gas/fumes/vapour/spray (appropriate wording to be specified by the manufacturer). Keep away from sources of ignition - No smoking. Provide for appropriate exhaust ventilation at places of vapours accumulation.
- Precautions for safe handling : Avoid breathing dust, fume, gas, mist, vapours, spray. Use only outdoors or in a well-ventilated area.
- Hygiene measures : Handle in accordance with good industrial hygiene and safety practice. Wash hands, forearms and face thoroughly after handling.

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

- Technical measures : Store in a well-ventilated place. Keep container tightly closed.
- Storage conditions : Store at room temperature away from light and moisture.

### 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

- Personal protective equipment : Gloves. Protective clothing. Protective goggles. Self-contained breathing apparatus.



- Materials for protective clothing : Wear suitable protective clothing and gloves.
- Hand protection : Wear suitable protective clothing and gloves.
- Eye protection : Wear eye protection. Chemical goggles or face shield with safety glasses.
- Skin and body protection : Wear suitable protective clothing.
- Respiratory protection : In case of inadequate ventilation wear respiratory protection. Approved supplied air respirator.

## SECTION 9: Physical and chemical properties

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

- Physical state : Liquid
- Appearance : Liquid.
- Molecular mass : 131.13 g/mol (Labeled)
- Colour : Colourless.
- Odour : No data available
- Odour threshold : No data available
- pH : No data available
- Relative evaporation rate (butylacetate=1) : No data available
- Melting point : -43 °C (-45 °F) - lit
- Freezing point : No data available
- Boiling point : 181 °C (358 °F) - lit
- Flash point : 85 °C (185 °F) - closed cup
- Auto-ignition temperature : 304 °C (579 °F)
- Decomposition temperature : No data available

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|                                  |                                       |
|----------------------------------|---------------------------------------|
| Flammability (solid, gas)        | : No data available                   |
| Vapour pressure                  | : 1 hPa (1 mmHg) at 28.5 °C (83.3 °F) |
| Relative vapour density at 20 °C | : No data available                   |
| Relative density                 | : No data available                   |
| Density                          | : 1.029 g/ml at 20 °C (68 °F) – lit.  |
| Solubility                       | : No data available                   |
| 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                   |
| Oxidising properties             | : No data available                   |
| Explosive limits                 | : 1.4 - 9.5 % (V)                     |

### 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 if stored under recommended conditions.

### 10.3. Possibility of hazardous reactions

No additional information available

### 10.4. Conditions to avoid

No additional information available

### 10.5. Incompatible materials

Acids. Bases. Oxidizing agent. Reducing agents.

### 10.6. Hazardous decomposition products

Carbon oxides (CO, CO<sub>2</sub>).

## SECTION 11: Toxicological information

### 11.1. Information on toxicological effects

Acute toxicity : Not classified

| ETHYL ACETOACETATE (3-13C, 99%) (144634-49-1) |                           |
|---|---------------------------|
| LD50 oral rat                                 | 3980 mg/kg                |
| ATE CLP (oral)                                | 3980.000 mg/kg bodyweight |

|   |   |
|---|---|
| Skin corrosion/irritation                           | : Causes skin irritation.<br>Skin - rabbit - Open irritation test   |
| Serious eye damage/irritation                       | : Causes serious eye irritation.<br>Eyes - rabbit - Moderate eye irritation - 24 h  |
| Respiratory or skin sensitisation                   | : Not available<br>No data available  |
| Germ cell mutagenicity                              | : Not available   |
| Carcinogenicity                                     | : Not classified  |
| Reproductive toxicity                               | : Not available   |
| STOT-single exposure                                | : May cause respiratory irritation.<br>No data available  |
| STOT-repeated exposure                              | : Not classified<br>No data available   |
| Aspiration hazard                                   | : Not classified  |
| Potential adverse human health effects and symptoms | : This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product. |
| Symptoms/injuries after inhalation                  | : May be harmful if inhaled. 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.

### SECTION 12: Ecological information

#### 12.1. Toxicity

Ecology - general : The product is not considered harmful to aquatic organisms nor to cause long-term adverse effects in the environment.

#### ETHYL ACETOACETATE (3-13C, 99%) (144634-49-1)

|                |   |
|----------------|---|
| LC50 fish 1    | Pimephales promelas (fathead minnow) - 96 h |
| EC50 Daphnia 1 | 646 mg/l Daphnia magna (Water flea) - 48 h  |

#### 12.2. Persistence and degradability

#### ETHYL ACETOACETATE (3-13C, 99%) (144634-49-1)

Persistence and degradability : Biodegradability: Result - Readily biodegradable.

#### 12.3. Bioaccumulative potential

#### ETHYL ACETOACETATE (3-13C, 99%) (144634-49-1)

Bioaccumulative potential : Not available.

#### 12.4. Mobility in soil

#### ETHYL ACETOACETATE (3-13C, 99%) (144634-49-1)

Ecology - soil : Not available.

#### 12.5. Results of PBT and vPvB assessment

No additional information available

#### 12.6. Other adverse effects

Other adverse effects : Not available.

### SECTION 13: Disposal considerations

#### 13.1. Waste treatment methods

Regional legislation (waste) : Waste materials should be disposed of under conditions which meet Federal, State, and Local environmental control regulations.  
Product/Packaging disposal recommendations: : Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.  
Ecology - waste materials : Dispose of as unused product.

### SECTION 14: Transport information

In accordance with ADR / RID / IMDG / IATA / ADN

#### 14.1. UN number

UN-No.(DOT) : 1993  
DOT NA no. : NA1993

#### 14.2. UN proper shipping name

Proper Shipping Name (DOT) : Combustible liquid, n.o.s.  
Class (DOT) : 3 - Class 3 - Flammable and combustible liquid 49 CFR 173.120  
DOT Symbols : D - Proper shipping name for domestic use only, or to and from Canada,G - Identifies PSN requiring a technical name  
Packing group (DOT) : III - Minor Danger  
DOT Special Provisions (49 CFR 172.102) : IB3 - Authorized IBCs: Metal (31A, 31B and 31N); Rigid plastics (31H1 and 31H2); Composite (31HZ1 and 31HA2, 31HB2, 31HN2, 31HD2 and 31HH2). Additional Requirement: Only liquids with a vapor pressure less than or equal to 110 kPa at 50 C (1.1 bar at 122 F), or 130 kPa at 55 C (1.3 bar at 131 F) are authorized, except for UN2672 (also see Special Provision IP8 in Table 2 for UN2672).  
T1 - 1.5 178.274(d)(2) Normal..... 178.275(d)(2)  
T4 - 2.65 178.274(d)(2) Normal..... 178.275(d)(3)  
TP1 - The maximum degree of filling must not exceed the degree of filling determined by the following: Degree of filling =  $97 / (1 + a (tr - tf))$  Where: tr is the maximum mean bulk temperature during transport, and tf is the temperature in degrees celsius of the liquid during filling.  
DOT Packaging Exceptions (49 CFR 173.xxx) : 150  
DOT Packaging Non Bulk (49 CFR 173.xxx) : 203  
DOT Packaging Bulk (49 CFR 173.xxx) : 241

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Marine pollutant : No

### 14.3. Additional information

Emergency Response Guide (ERG) Number : 128  
Other information : No supplementary information available.  
Special transport precautions : IMDG/IATA: Not dangerous goods.

#### Overland transport

Packing group (ADR) : III  
Class (ADR) : 3 - Flammable liquid  
Hazard identification number (Kemler No.) : 33  
Classification code (ADR) : F1  
Danger labels (ADR) : 3 - Flammable liquids



Orange plates :

Tunnel restriction code (ADR) : D/E  
Limited quantities (ADR) : 5l  
EAC code : •3YE  
Excepted quantities (ADR) : E1

#### Transport by sea

DOT Vessel Stowage Location : A - The material may be stowed "on deck" or "under deck" on a cargo vessel and on a passenger vessel.  
MFAG-No : 127;128

#### Air transport

DOT Quantity Limitations Passenger aircraft/rail (49 CFR 173.27) : 60 L  
DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75) : 220 L  
Civil Aeronautics Law : Flammable liquids

### 14.4. Environmental hazards

Other information : No supplementary information available.

### 14.5. Special precautions for user

Special transport precautions : IMDG/IATA: Not dangerous goods.

### 14.6. Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable

## SECTION 15: Regulatory information

### 15.1. US Federal regulations

| ETHYL ACETOACETATE (3-13C, 99%) (144634-49-1)      |  |
|--|--|
| SARA Section 302 Threshold Planning Quantity (TPQ) | Not subject to reporting requirements of the United States SARA Section 302. |
| SARA Section 311/312 Hazard Classes                | Fire hazard<br>Immediate (acute) health hazard                               |
| SARA Section 313 - Emission Reporting              | Not subject to reporting requirements of the United States SARA Section 313. |

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### 15.2. International regulations

#### CANADA

##### ETHYL ACETOACETATE (3-13C, 99%) (144634-49-1)

Listed on the Canadian DSL (Domestic Substances List)

#### 15.2.1. National regulations

No additional information available

### 15.3. US State regulations

##### ETHYL ACETOACETATE (3-13C, 99%)(144634-49-1)

|   |   |
|---|---|
| U.S. - California - Proposition 65 - Carcinogens List               | No  |
| 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  |
| State or local regulations  | U.S. - Massachusetts - Right To Know List<br>U.S. - Pennsylvania - RTK (Right to Know) List<br>U.S. - New Jersey - Right to Know Hazardous Substance List |

## SECTION 16: Other information

Other information : This product is not radioactive. The data given for this product are those of the corresponding unlabeled compound, unless specifically indicated otherwise. Health and safety data for labeled compounds are generally not available, but are assumed to be similar or identical to the corresponding unlabeled compound.

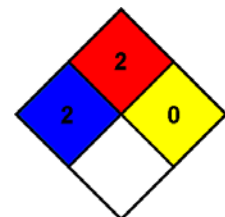
Full text of R-, H- and EUH-statements:

|               |  |
|---------------|--|
| Eye Irrit. 2  | Serious eye damage/eye irritation, Category 2  |
| Skin Irrit. 2 | Skin corrosion/irritation, Category 2  |
| STOT SE 3     | Specific target organ toxicity — Single exposure, Category 3, Respiratory tract irritation |
| H315          | Causes skin irritation   |
| H319          | Causes serious eye irritation  |
| H335          | May cause respiratory irritation   |
| R36/37/38     | Irritating to eyes, respiratory system and skin  |
| Xi            | Irritant   |

NFPA health hazard : 2 - Materials that, under emergency conditions, can cause temporary incapacitation or residual injury.

NFPA fire hazard : 2 - Materials that must be moderately heated or exposed to relatively high ambient temperatures before ignition can occur.

NFPA reactivity : 0 - Material that in themselves are normally stable, even under fire conditions.



### HMIS III Rating

Health : 2 Moderate Hazard - Temporary or minor injury may occur

Flammability : 2 Moderate Hazard

Physical : 0 Minimal Hazard

CIL Multi-Solvent Mixture SDS

*This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product*