



ETHYL ACETOACETATE (1,3-13C2, 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

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Supersedes: 01/01/2012

Version: 3.0

CLM-522

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

1.1. Product identifier

Product form : Substance
Substance name : ETHYL ACETOACETATE (1,3-13C2, 99%)
EC No : 205-516-1 (Unlabeled)
CAS No : 77504-73-5
Product code : CLM-522
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 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 dust, fume, gas, mist, spray, vapours
P264 - Wash hands, forearms and face thoroughly after handling
P271 - Use only outdoors or in a well-ventilated area
P280 - Wear 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

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, fume, gas, mist, spray, vapours
P264 - Wash hands, forearms and face thoroughly after handling
P271 - Use only outdoors or in a well-ventilated area
P280 - Wear 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 (CO₂), 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 (1,3-13C2, 99%)	(CAS No) 77504-73-5 (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 (1,3-13C2, 99%)	(CAS No) 77504-73-5 (EC No) 205-516-1 (Unlabeled)	100	Skin Irrit. 2, H315 Eye Irrit. 2, H319 STOT SE 3, H335

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

Name	Product identifier	%	GHS-US classification
ETHYL ACETOACETATE (1,3-13C2, 99%) (Main constituent)	(CAS No) 77504-73-5	100	Flam. Liq. 4, H227 Skin Irrit. 2, H315 Eye Irrit. 2A, H319 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 off with soap and plenty of water. Consult a physician. 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 (CO2).

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

Precautions for safe handling : Avoid breathing dust, fume, gas, mist, spray, vapours. Use only outdoors or in a well-ventilated area. Avoid contact with skin and eyes. Eliminate all ignition sources if safe to do so. Ensure good ventilation of the work station. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Take precautionary measures against static discharge.

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 tightly closed in a dry and cool place.

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. Self-contained breathing apparatus. Protective goggles.



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, gloves and eye/face protection.

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 : 132.13 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 : 73.5 °C (164.3 °F) - closed cup
Auto-ignition temperature : 304 °C (579 °F)
Decomposition temperature : No data available
Flammability (solid, gas) : No data available

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Vapour pressure	: 0.26 hPa (.20 mmHg) at 20 °C (68 °F) - OECD Test Guideline 104
Vapour pressure at 50 °C	: 3.5 hPa (2.6 mmHg) at 50 °C (122 °F) - OECD Test Guideline 104
Relative vapour density at 20 °C	: 4.49 (Air = 1.0)
Relative density	: No data available
Density	: 1.029 g/ml at 20 °C (68 °F) - lit.
Solubility	: Water: 130 g/l at 20 °C (68 °F) - OECD Test Guideline 105
Log Pow	: 0.8 at 20 °C (68 °F) - OECD Test Guideline 117
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, CO2).

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity : Not classified

ETHYL ACETOACETATE (1,3-13C2, 99%) (77504-73-5)	
LD50 oral rat	10800 mg/kg female
LD50 dermal rat	> 2000 male and female - OECD Guideline 402
ATE CLP (oral)	3980.000 mg/kg bodyweight

Skin corrosion/irritation	: Causes skin irritation. Skin - rabbit - Open irritation test
Serious eye damage/irritation	: Causes serious eye irritation. Eyes - rabbit - Moderate eye irritation - 24 h
Respiratory or skin sensitisation	: Not available No data available
Germ cell mutagenicity	: Not available
Carcinogenicity	: Not classified
Reproductive toxicity	: Not available
STOT-single exposure	: May cause respiratory irritation. No data available
STOT-repeated exposure	: Not classified 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.

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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.

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 (1,3-13C2, 99%) (77504-73-5)

LC50 fish 1	> 100 mg/l semi static test - Danio rerio (zebra fish) - 96 h
EC50 Daphnia 1	> 100 mg/l semi static test - Daphnia magna (Water flea) - 48 h
EC50 other aquatic organisms 1	> 100 ml/l semi static test - Desmodesmus subspicatus (green algae) - 72 h

12.2. Persistence and degradability

ETHYL ACETOACETATE (1,3-13C2, 99%) (77504-73-5)

Biodegradation	66 % Readily biodegradable
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12.3. Bioaccumulative potential

ETHYL ACETOACETATE (1,3-13C2, 99%) (77504-73-5)

Log Pow	0.8 at 20 °C (68 °F) - OECD Test Guideline 117
Bioaccumulative potential	Not available.

12.4. Mobility in soil

ETHYL ACETOACETATE (1,3-13C2, 99%) (77504-73-5)

Ecology - soil	Not available.
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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.

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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
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

No additional information available

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.

Air transport

DOT Quantity Limitations Passenger aircraft/rail : 60 L
(49 CFR 173.27)
DOT Quantity Limitations Cargo aircraft only (49 : 220 L
CFR 175.75)

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 (1,3-13C2, 99%) (77504-73-5)	
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 Immediate (acute) health hazard
SARA Section 313 - Emission Reporting	Not subject to reporting requirements of the United States SARA Section 313.

15.2. International regulations

CANADA

ETHYL ACETOACETATE (1,3-13C2, 99%) (77504-73-5)
Listed on the Canadian DSL (Domestic Substances List)

15.2.1. National regulations

No additional information available

15.3. US State regulations

ETHYL ACETOACETATE (1,3-13C2, 99%)(77504-73-5)	
U.S. - California - Proposition 65 - Carcinogens List	No
U.S. - California - Proposition 65 - Developmental Toxicity	No
U.S. - California - Proposition 65 - Reproductive	No

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Toxicity - Female	
U.S. - California - Proposition 65 - Reproductive Toxicity - Male	No
State or local regulations	U.S. - Massachusetts - Right To Know List U.S. - Pennsylvania - RTK (Right to Know) List 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.

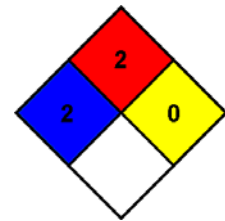
Full text of R-, H- and EUH-statements:

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