

Methyl acetoacetate SDS/MSDS (Safety Data Sheet)

1. PRODUCT AND COMPANY IDENTIFICATION

Product identifier

- * Product Name: Methyl acetoacetate
- * Catalog Number: S3091
- * CAS Number: 105-45-3
- * IUPAC Name: Butanoic acid, 3-oxo-, methyl ester

Relevant identified uses and uses advised against

- * Identified uses: For research and development use only; laboratory chemicals; manufacture of substances.
- * Uses advised against: Not for pharmaceutical, household, or other unapproved uses.

Details of the supplier

- * Company: Selleck Chemicals
- * TollFree: +1 877 796-6397
- * Tel: +1 832 582-8158
- * Fax: +1 832 582-8590

Emergency telephone number

- * Emergency phone #: +1 832 582-8158

2. HAZARDS IDENTIFICATION

2.1 GHS classification in accordance with 29 CFR 1910 (OSHA HCS):

- Flammable liquids: Category 4. H227
- Serious eye irritation: Category 2. H319
- Specific target organ toxicity (single exposure): Category 3. H336

2.2 GHS Label elements, including precautionary statements

Hazard Pictogram(s)



Signal Word

Warning

Hazard statement(s)

H227: Combustible liquid
H319: Causes serious eye irritation
H336: May cause drowsiness or dizziness

Precautionary statement(s)

None.

Prevention	P210: Keep away from heat, hot surface, sparks, open flames and other ignition sources. No smoking. P261: Avoid breathing dust/fume/gas/mist/vapors/spray. P264+P265: Wash hands thoroughly after handling. Do not touch eyes. P271: Use only outdoors or in a well-ventilated area. P280: Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.
Response	P304+P340: IF INHALED: Remove person to fresh air and keep comfortable for breathing. P305+P351: IF IN EYES: Rinse cautiously with water for several minutes. P319: Get medical help if you feel unwell. P337+P317: If eye irritation persists: Get medical help. P338: Remove contact lenses, if present and easy to do. Continue rinsing. P370+P378: In case of fire: Use water spray, dry chemical, carbon dioxide, or appropriate foam to extinguish.
Storage	P403: Store in a well-ventilated place. P403+P233: Store in a well-ventilated place. Keep container tightly closed. P405: Store locked up.
Disposal	P501: P501 Dispose of contents/ container to an approved waste disposal plant.

2.3 Other hazards

None.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Product name: Methyl acetoacetate

CAS Number: 105-45-3

PubChem CID: 7757

3.2 Mixtures

Not applicable (pure substance).

4. FIRST-AID MEASURES

4.1 Description of first aid measures

Inhalation: Fresh air, rest. Refer for medical attention.

Skin contact: Remove contaminated clothes. Rinse skin with plenty of water or shower.

Eye contact: First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

Ingestion: Rinse mouth. Do NOT induce vomiting. Give one or two glasses of water to drink. Refer for medical attention .

4.2 Most important symptoms and effects, both acute and delayed

See Section 11 (Toxicological Information).

4.3 Indication of any immediate medical attention and special treatment needed

Treat symptomatically. Contact a poison control center or physician for severe exposure.

5. FIRE-FIGHTING MEASURES

5.1 Extinguishing media

Suitable: Water spray, dry chemical, carbon dioxide (CO₂), alcohol-resistant foam.

Unsuitable: None known.

5.2 Specific hazards arising from the substance or mixture

Excerpt from ERG Guide 128 [Flammable Liquids (Water-Immiscible)]:

CAUTION: The majority of these products have a very low flash point. Use of water spray when fighting fire may be inefficient. CAUTION: For mixtures containing alcohol or polar solvent, alcohol-resistant foam may be more effective.

SMALL FIRE: Dry chemical, CO₂, water spray or regular foam. If regular foam is ineffective or unavailable, use alcohol-resistant foam.

LARGE FIRE: Water spray, fog or regular foam. If regular foam is ineffective or unavailable, use alcohol-resistant foam. Avoid aiming straight or solid streams directly onto the product. If it can be done safely, move undamaged containers away from the area around the fire.

FIRE INVOLVING TANKS, RAIL TANK CARS OR HIGHWAY TANKS: Fight fire from maximum distance or use unmanned master stream devices or monitor nozzles. Cool containers with flooding quantities of water until well after fire is out. For petroleum crude oil, do not spray water directly into a breached tank car. This can lead to a dangerous boil over. Withdraw immediately in case of rising sound from venting safety devices or discoloration of tank. ALWAYS stay away from tanks in direct contact with flames. For massive fire, use unmanned master stream devices or monitor nozzles; if this is impossible, withdraw from area and let fire burn. (ERG, 2024)

Use alcohol-resistant foam, powder, carbon dioxide.

... /Use/ foam, carbon dioxide, dry chemical.

If material on fire or involved in fire: Do not extinguish fire unless flow can be stopped. Use water in flooding quantities as fog. Solid streams of water may be ineffective. Cool all affected containers with flooding quantities of water. Apply water from as far a distance as possible. Use "alcohol" foam, dry chemical or carbon dioxide.

5.3 Advice for firefighters

Wear self-contained breathing apparatus (SCBA) and full protective clothing.

Fight fire from upwind. Cool containers with water spray until fire is extinguished.

Flash point: 158 °F (USCG, 1999)

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Wear appropriate personal protective equipment (see Section 8).

Avoid breathing dust/vapor. Ensure adequate ventilation.

Evacuate personnel to safe areas. Keep people away from and upwind of spill.

6.2 Environmental precautions

Prevent product from entering drains, waterways, or soil.

Contain spill with inert absorbent material.

6.3 Methods and materials for containment and cleaning up

Excerpt from ERG Guide 128 [Flammable Liquids (Water-Immiscible)]:

IMMEDIATE PRECAUTIONARY MEASURE: Isolate spill or leak area for at least 50 meters (150 feet) in all directions.

LARGE SPILL: Consider initial downwind evacuation for at least 300 meters (1000 feet).

FIRE: If tank, rail tank car or highway tank is involved in a fire, ISOLATE for 800 meters (1/2 mile) in all directions; also, consider initial evacuation for 800 meters (1/2 mile) in all directions. (ERG, 2024)

Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Ventilation. Collect leaking and spilled liquid in sealable containers as far as possible. Wash away remainder with plenty of water.

SRP: The most favorable course of action is to use an alternative chemical product with less inherent propensity for occupational exposure or environmental contamination. Recycle any unused portion of the material for its approved use or return it to the manufacturer or supplier. Ultimate disposal of the chemical must consider: the material's impact on air quality; potential migration in soil or water; effects on animal, aquatic, and plant life; and conformance with environmental and public health regulations.

If material not on fire and not involved in fire: Keep sparks, flames, and other sources of ignition away. Keep material out of water sources and sewers. Build dikes to contain flow as necessary. Use water spray to knock-down vapors.

Personnel protection: Avoid breathing vapors. Keep upwind. ... Do not handle broken packages unless wearing appropriate personal protective equipment. Wash away any material which may have contacted the body with copious amounts of water or soap and water.

SRP: The scientific literature for the use of contact lenses in industry is conflicting. The benefit or detrimental effects of wearing contact lenses depend not only upon the substance, but also on factors including the form of the substance, characteristics and duration of the exposure, the uses of other eye protection equipment, and the hygiene of the lenses. However, there may be individual substances whose irritating or corrosive properties are such that the wearing of contact lenses would be harmful to the eye. In those specific cases, contact lenses should not be worn. In any event, the usual eye protection equipment should be worn even when contact lenses are in place.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Excerpt from ERG Guide 128 [Flammable Liquids (Water-Immiscible)]:

ELIMINATE all ignition sources (no smoking, flares, sparks or flames) from immediate area. All equipment used when handling the product must be grounded. Do not touch or walk through spilled material. Stop leak if you can do it without risk. Prevent entry into waterways, sewers, basements or confined areas. A vapor-suppressing foam may be used to reduce vapors. Absorb or cover with dry earth, sand or other non-combustible material and transfer to containers. Use clean, non-sparking tools to collect absorbed material.

LARGE SPILL: Dike far ahead of liquid spill for later disposal. Water spray may reduce vapor, but may not prevent ignition in closed spaces. (ERG, 2024)

Separated from oxidants.

7.2 Conditions for safe storage, including any incompatibilities

Separated from oxidants.

Store away from incompatible materials (see Section 10).

[Note: Specific storage temperature not available in public databases. Refer to supplier Certificate of Analysis (COA) for exact storage conditions.]

Store in original container. Keep upright to prevent leakage.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Exposure controls

8.1.1 Occupational exposure limits (OEL)

OSHA PEL: Not established.

ACGIH TLV: Not established.

NIOSH REL: Not established.

No occupational exposure limit values are established for this substance.

Use the lowest feasible exposure level (ALARA principle).

8.1.2 Appropriate engineering controls

Use only in a chemical fume hood or with local exhaust ventilation.

Ensure adequate ventilation to keep airborne concentrations below exposure limits.

8.2 Individual protection measures

8.2.1 Eye/face protection

Wear chemical safety goggles.

8.2.2 Skin protection

Wear protective gloves. Recommended material: Nitrile rubber.

Wear suitable protective clothing (lab coat).

8.2.3 Respiratory protection

Use NIOSH-approved dust/mist respirator (N95 or higher) if ventilation is inadequate.

8.2.4 Thermal hazards

Not applicable.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a) Appearance: Methyl acetoacetate appears as a clear colorless liquid. Flash point 158 °F. Denser than water and slightly soluble in water. Vapors heavier than air.

b) Odor: Agreeable odor

c) Odor threshold: No data available

d) pH: No data available

e) Melting point/freezing point: -112 °F (USCG, 1999)

f) Initial boiling point and boiling range: 336 to 338 °F at 760 mmHg (USCG, 1999)

g) Flash point: 158 °F (USCG, 1999)

h) Evaporation rate: No data available

i) Flammability (solid, gas): No data available

j) Upper/lower flammability or explosive limits: No data available

k) Vapor pressure: 0.89 [mmHg]

l) Vapor density: No data available

m) Relative density: 1.076 (USCG, 1999) - Denser than water; will sink

n) Water solubility: Soluble in 2 parts water; miscible with alcohol and ether

o) Partition coefficient: n-octanol/water: Log P: No data available

p) Auto-ignition temperature: 536 °F (USCG, 1999)

q) Decomposition temperature: No data available

r) Viscosity: 1.704 cPa at 20 °C

s) Explosive properties: No data available

t) Oxidizing properties: No data available

9.2 Other information

10. STABILITY AND REACTIVITY

10.1 Reactivity

No specific reactivity hazards identified under normal handling conditions.

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

No hazardous reactions under normal conditions.

10.4 Conditions to avoid

Avoid heat, sparks, open flames, direct sunlight, and moisture.

10.5 Incompatible materials

Strong oxidizing agents, strong acids, strong bases.

10.6 Hazardous decomposition products

No data available.

See also Section 5 (Fire-fighting measures) for combustion products.

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity:

No acute toxicity data available.

Skin corrosion/irritation:

No data available.

Serious eye damage/eye irritation:

Causes serious eye irritation (H319).

Respiratory or skin sensitization:

No data available.

Germ cell mutagenicity:

No data available.

Carcinogenicity:

No data available.

Reproductive toxicity:

No data available.

Specific target organ toxicity (single exposure):

No data available.

Specific target organ toxicity (repeated exposure):

No data available.

Aspiration hazard:

No data available.

11.2 Additional information

Exposure routes:

The substance can be absorbed into the body by inhalation of its vapour.

Signs and symptoms of exposure:

Cough. Dizziness. Drowsiness. Headache. Sore throat.

Redness. Pain.

Data source: Hazardous Substances Data Bank (HSDB) via PubChem.

12. ECOLOGICAL INFORMATION

12.1 Toxicity

EC50 *Daphnia magna* (Water flea; Acute immobilization test and reproduction) >236.9 mg/L/48 hr; static; exposure temperature ranged from 20-21 °C, pH ranged from 7.9 to 8.3, and dissolved oxygen ranged from 8.7 to 8.9 mg/L
LC50 *Pimephales promelas* (Fathead minnow) >111.4 mg/L/96 hr; static; temperature ranged from 19-20 °C, pH ranged from 7.7 to 8.4 and dissolved oxygen ranged from 7.8 to 9.1 mg/L.

EC50 *Selenastrum capricornutum* (cell growth rate) >978.0 mg/L/24 hr, 48 hr, 72 hr /Conditions of bioassay not specified in source examined/

Methyl acetoacetate's production and use as a solvent for cellulose ethers and esters and in organic synthesis may result in its release to the environment through various waste streams. Methyl acetoacetate was found in the condensed smoke of fires of ponderosa pine sapwood, needles, bark, litter, duff, and humus. If released to air, a vapor pressure of 0.892 mm Hg at 25 °C indicates methyl acetoacetate will exist solely as a vapor in the ambient atmosphere. Vapor-phase methyl acetoacetate will be degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 5 days. If released to soil, methyl acetoacetate is expected to have very high mobility based upon an estimated Koc of 1.0. Volatilization from moist soil surfaces is expected to be slow based upon an estimated Henry's Law constant of 2.7×10^{-7} atm-cu m/mole. Methyl acetoacetate is not expected to volatilize fr

12.2 Persistence and degradability

No data available.

12.3 Bioaccumulative potential

No data available.

12.4 Mobility in soil

No data available.

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available.

12.6 Other adverse effects

No other adverse ecological effects identified.

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Waste Treatment Methods: Waste material must be disposed of in accordance with national and local regulations. Leave chemicals in original containers and do not mix with other waste. Handle uncleaned containers in the same manner as the product itself.

14. TRANSPORT INFORMATION**14.1 UN number**

Not regulated as dangerous goods (research quantities typically exempt).

14.2 UN proper shipping name

Not subject to transport regulations (small quantities for research use).

14.3 Transport hazard class(es)

Not classified as dangerous goods for transport (research quantities).

DOT label: Combustible Liquid

14.4 Packing group

Not applicable (not regulated as dangerous goods in typical research quantities).

14.5 Environmental hazards

Marine pollutant: No (not classified as environmentally hazardous per GHS).

14.6 Special precautions for user

Transport in original packaging. Ensure containers are tightly sealed.

For bulk or commercial quantities, consult applicable transport regulations (DOT, IATA, IMDG).

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

Not applicable.

15. REGULATORY INFORMATION**15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture**

US EPA / TSCA: Subject to EPA TSCA regulations

EU ECHA / REACH: Registered (REACH Active)

SARA 302 Components:

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components:

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards:

Acute (short-term) health hazard

Fire hazard

Massachusetts Right To Know Components:

This material contains components subject to the Massachusetts Right to Know Act. See Section 2 for hazard classification.

Pennsylvania Right To Know Components:

This material contains components subject to the Pennsylvania Right to Know Act. See Section 2 for hazard classification.

New Jersey Right To Know Components:

This material contains components subject to the New Jersey Right to Know Act. See Section 2 for hazard classification.

California Prop. 65 Components:

This product does not contain any chemicals known to the State of California to cause cancer, birth defects, or any other reproductive harm.

Other regulatory listings:

- The Australian Inventory of Industrial Chemicals: Chemical: Butanoic acid, 3-oxo-, methyl ester
- EFSA Legal Basis: Commission Regulation (EC) No 1565/2000 (Repealed by Com. Implementing Reg. (EU) No 872/2012)
- Atmospheric Standards: This action promulgates standards of performance for equipment leaks of Volatile Organic Compounds (VOC) in the Synthetic Organic Chemical Manufacturing Industry (SOCMI). The intended effect of these standards is to require all newly constructed, modified, and reconstructed SOCMI process units to us

15.2 Chemical safety assessment

A chemical safety assessment has not been carried out for this substance.

For research-use-only compounds, no CSA is required under REACH Annex I.

16. OTHER INFORMATION

Revision Date: 2026/09/09

Further Information: The information provided is believed to be correct but is not exhaustive and should be used only as a guideline based on current knowledge. It does not represent a guarantee of the properties of the product.

Selleck Chemicals Corporation and its Affiliates shall not be held liable for any damage resulting from handling or contact with the product.