

Material Safety Data Sheet

HAZARD WARNINGS	RISK PHRASES	PROTECTIVE CLOTHING
	Combustible material; avoid heat and sources of ignition. Irritating to skin, eyes, and the respiratory system.	

Section I. Chemical Product and Company Identification

Chemical Name	Methyl Acetoacetate		
Catalog Number	A0650	Supplier	TCI America 9211 N. Harborgate St. Portland OR 1-800-423-8616
Synonym	3-Oxobutyric Acid Methyl Ester; Methyl 3-Oxobutyrate; Acetoacetic Acid Methyl Ester		
Chemical Formula	C ₅ H ₈ O ₃		
CAS Number	105-45-3	In case of Emergency Call	Chemtrec® (800) 424-9300 (U.S.) (703) 527-3887 (International)

Section II. Composition and Information on Ingredients

Chemical Name	CAS Number	Percent (%)	TLV/PEL	Toxicology Data
Methyl Acetoacetate	105-45-3	Min. 99.0 (GC)	Not available.	Rat LD ₅₀ (oral) 2.58 gm/kg

Section III. Hazards Identification

Acute Health Effects	Irritating to eyes and skin on contact. Inhalation causes irritation of the lungs and respiratory system. Inflammation of the eye is characterized by redness, watering, and itching. Skin inflammation is characterized by itching, scaling, reddening, or, occasionally, blistering. Follow safe industrial hygiene practices and always wear proper protective equipment when handling this compound.
Chronic Health Effects	CARCINOGENIC EFFECTS : Not available. MUTAGENIC EFFECTS : Not available. TERATOGENIC EFFECTS : Not available. DEVELOPMENTAL TOXICITY : Not available. Repeated or prolonged exposure to this compound is not known to aggravate existing medical conditions.

Section IV. First Aid Measures

Eye Contact	Check for and remove any contact lenses. In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Get medical attention.
Skin Contact	In case of contact, immediately flush skin with plenty of water. Remove contaminated clothing and shoes. Wash clothing before reuse. Thoroughly clean shoes before reuse. Get medical attention.
Inhalation	If the victim is not breathing, perform mouth-to-mouth resuscitation. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, oxygen can be administered. Seek medical attention if respiration problems do not improve.
Ingestion	INDUCE VOMITING by sticking finger in throat. Lower the head so that the vomit will not reenter the mouth and throat. Loosen tight clothing such as a collar, tie, belt or waistband. If the victim is not breathing, perform mouth-to-mouth resuscitation. Examine the lips and mouth to ascertain whether the tissues are damaged, a possible indication that the toxic material was ingested; the absence of such signs, however, is not conclusive.

Section V. Fire and Explosion Data

Flammability	Combustible.	Auto-Ignition	280 °C (536 °F)
Flash Points	72 °C (161.6 °F)	Flammable Limits	LOWER: 1.4 to 3.1% UPPER: 14.5 to 16%
Combustion Products	These products are toxic carbon oxides (CO, CO ₂).		
Fire Hazards	Not available.		
Explosion Hazards	Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available.		
Fire Fighting Media and Instructions	SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use water spray, fog or foam. DO NOT use water jet. Consult with local fire authorities before attempting large scale fire-fighting operations.		

Section VI. Accidental Release Measures

Spill Cleanup Instructions Combustible material. Irritating material. Keep away from heat. Mechanical exhaust required. Stop leak if without risk. Absorb with an inert material and put the spilled material in an appropriate waste disposal. Consult federal, state, and/or local authorities for assistance on disposal.

Section VII. Handling and Storage

Handling and Storage Information COMBUSTIBLE. IRRITANT. Keep away from heat. Mechanical exhaust required. Avoid excessive heat and light. Do not breathe gas/fumes/ vapor/spray. Always store away from incompatible compounds such as oxidizing agents.

Section VIII. Exposure Controls/Personal Protection

Engineering Controls Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapors below their respective threshold limit value. Ensure that eyewash station and safety shower is proximal to the work-station location.

Personal Protection Splash goggles. Lab coat. Vapor respirator. Boots. Gloves. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product. Be sure to use a MSHA/NIOSH approved respirator or equivalent.



Exposure Limits Not available.

Section IX. Physical and Chemical Properties

Physical state @ 20°C	Liquid. (Clear, colorless.)	Solubility	Soluble in alcohol, ether, and other organic solvents. Fully miscible with water.
Specific Gravity	1.08 (water=1)		
Molecular Weight	116.12	Partition Coefficient	LOG P _{ow} : -0.26
Boiling Point	170°C (338°F)	Vapor Pressure	0.17 kPa (@ 20°C)
Melting Point	-80°C (-112°F)	Vapor Density	4.0 (Air = 1)
Refractive Index	1.42	Volatility	Not available.
Critical Temperature	Not available.	Odor	Characteristic.
Viscosity	Not available.	Taste	Not available.

Section X. Stability and Reactivity Data

Stability This material is stable if stored under proper conditions. (See Section VII for instructions)

Conditions of Instability Avoid excessive heat and light.

Incompatibilities Reactive with oxidizing agents.

Section XI. Toxicological Information

RTECS Number AK5775000

Routes of Exposure Eye Contact. Ingestion. Inhalation.

Toxicity Data Rat LD₅₀ (oral) 2.58 gm/kg

Chronic Toxic Effects **CARCINOGENIC EFFECTS** : Not available.
MUTAGENIC EFFECTS : Not available.
TERATOGENIC EFFECTS : Not available.
DEVELOPMENTAL TOXICITY: Not available.
Repeated or prolonged exposure to this compound is not known to aggravate existing medical conditions.

Acute Toxic Effects Irritating to eyes and skin on contact. Inhalation causes irritation of the lungs and respiratory system. Inflammation of the eye is characterized by redness, watering, and itching. Skin inflammation is characterized by itching, scaling, reddening, or, occasionally, blistering.
Follow safe industrial hygiene practices and always wear proper protective equipment when handling this compound.

Section XII. Ecological Information

Ecotoxicity Not available.

Environmental Fate 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 deg 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 K_{oc} of 1.0. Volatilization from moist soil surfaces is expected to be slow based upon an estimated Henry's Law constant of 2.7X10⁻⁷ atm-cu m/mole. Methyl acetoacetate is not expected to volatilize from dry soil surfaces based upon its vapor pressure. One screening test observed 90% biodegradation of methyl acetoacetate in 2 days; although this study was not specific to soil, it suggests that biodegradation in soil and water may be rapid. If released into water, methyl

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Emergency phone number (800) 424-9300

acetoacetate is not expected to adsorb to suspended solids and sediment based upon the estimated K_{oc} . Volatilization from water surfaces is expected to be slow based upon this compound's estimated Henry's Law constant. An estimated BCF of 3.1 suggests the potential for bioconcentration in aquatic organisms is low. Methyl acetoacetate does not absorb light with wavelengths 290 nm and is not expected to be susceptible to direct photolysis by sunlight. Based on an estimated base-catalyzed second-order hydrolysis rate constant of 0.57 L/mole-sec, half-lives of 140 and 14 days at pH values of 7 and 8 can be calculated for methyl acetoacetate, respectively. Methyl acetoacetate would be expected to undergo hydrolysis in environmental waters and moist soils under basic conditions. Occupational exposure to methyl acetoacetate may occur through inhalation and dermal contact with this compound at workplaces where methyl acetoacetate is produced or used. The general population may be exposed to methyl acetoacetate via inhalation of ambient air containing wood smoke.

Section XIII. Disposal Considerations

Waste Disposal Recycle to process, if possible. Consult your local regional authorities. You may be able to dissolve or mix material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber system. Observe all federal, state and local regulations when disposing of the substance.

Section XIV. Transport Information

DOT Classification Not a DOT controlled material (United States).

PIN Number Not applicable.

Proper Shipping Name Not applicable.

Packing Group (PG) Not applicable.

DOT Pictograms



Section XV. Other Regulatory Information and Pictograms

TSCA Chemical Inventory (EPA) This compound is **ON** the EPA Toxic Substances Control Act (TSCA) inventory list.

WHMIS Classification (Canada) CLASS B-3: Combustible liquid with a flash point between 37.8°C (100°F) and 93.3°C (200°F).
On DSL.

EINECS Number (EEC) 203-299-8

EEC Risk Statements R36/37/38- Irritating to eyes, respiratory system and skin.

Japanese Regulatory Data ENCS No. 2-1474; 2-1475; 2-1505

Section XVI. Other Information

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Notice to Reader

TCI laboratory chemicals are for research purposes only and are NOT intended for use as drugs, food additives, households, or pesticides. The information herein is believed to be correct, but does not claim to be all inclusive and should be used only as a guide. Neither the above named supplier nor any of its subsidiaries assumes any liability whatsoever for the accuracy or completeness of the information contained herein. Final determination of suitability of any material is the sole responsibility of the user. All chemical reagents must be handled with the recognition that their chemical, physiological, toxicological, and hazardous properties have not been fully investigated or determined. All chemical reagents should be handled only by individuals who are familiar with their potential hazards and who have been fully trained in proper safety, laboratory, and chemical handling procedures. Although certain hazards are described herein, we can not guarantee that these are the only hazards which exist. Our MSDS sheets are based only on data available at the time of shipping and are subject to change without notice as new information is obtained. Avoid long storage periods since the product is subject to degradation with age and may become more dangerous or hazardous. It is the responsibility of the user to request updated MSDS sheets for products that are stored for extended periods. Disposal of unused product must be undertaken by qualified personnel who are knowledgeable in all applicable regulations and follow all pertinent safety precautions including the use of appropriate protective equipment (e.g. protective goggles, protective clothing, breathing equipment, facial mask, fume hood). For proper handling and disposal, always comply with federal, state, and local regulations.