

Product Data Sheet

Product Name: Ethyl 2-acetoxy-2-methylacetoacetate

Cat. No.: GF13011

Chemical Properties

Cas. No. 25409-39-6

Formula $C_9H_{14}O_5$

M.Wt 202.2

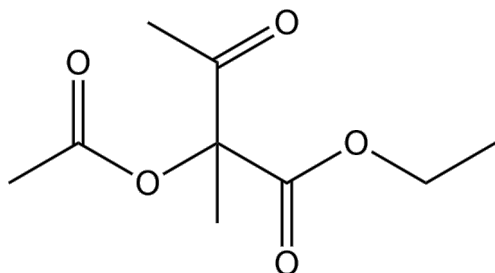
Solubility

Storage 2-8°C

General tips For obtaining a higher solubility, please warm the tube at 37 °C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution : ship with blue ice All other available size: ship with RT, or blue ice upon request.

Structure



Protocol

This protocol uses the experiment of synthesizing 2-levulinic acid using Ethyl 2-acetoxy-2-methylacetoacetate^[1-2] as an example. It is only used as an experimental guide. The actual application needs to be modified according to your needs.

1. Reagent preparation: Ethyl 2-acetoxy-2-methylacetoacetate; sulfuric acid (H_2SO_4 , 10%); sodium bicarbonate ($NaHCO_3$, saturated solution); anhydrous magnesium sulfate ($MgSO_4$, desiccant); ether (extraction solvent).

2. Acidic hydrolysis: Add Ethyl 2-acetoxy-2-methylacetoacetate (5.0g, about 24mmol) and 10% H_2SO_4 (30mL) to a 100mL round-bottom flask in sequence and shake to mix. Connect the round-bottom flask to a reflux condenser, heat to 80-90°C, and stop heating after stirring for 4-6 hours. The reaction mixture was cooled to room temperature, the product was extracted with ether (3×20mL), and the organic phases were combined. The organic phase was washed with saturated $NaHCO_3$ solution until neutral. After drying with anhydrous $MgSO_4$, the solvent was removed by rotary evaporation after filtration to obtain a crude product.

Caution: Product has not been fully validated for medical applications. For research use only.

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3. Decarboxylation reaction: The crude product was dissolved in a small amount of water, heated to 100°C for 1-2 hours to promote the release of CO₂. After cooling, it was extracted again with ether, dried and concentrated to obtain 2-levulinic acid.

4. Purification and storage: 2-levulinic acid was distilled under reduced pressure, and the fraction with a boiling point of 120-130°C/10mmHg was collected, dissolved in hot ethanol, cooled and crystallized, and filtered and dried to obtain the pure product. The pure product was sealed and stored at 4°C (short term) or -20°C (long term) in a light-proof manner to avoid moisture absorption.

Precautions:

1. Protective equipment (gloves, goggles) must be worn when operating under strong acid conditions.
2. Heat slowly during the decarboxylation stage to avoid violent boiling.
3. For your safety and health, please wear a lab coat and disposable gloves when operating.
4. Avoid inhaling vapors and operate in a fume hood.

References:

- [1]. Dulieu C, Poncelet D. Spectrophotometric assay of α -acetolactate decarboxylase. Enzyme and microbial technology. 1999 Sep 1;25(6):537-42.
- [2]. Park SH, Xing R, Whitman WB. Nonenzymatic acetolactate oxidation to diacetyl by flavin, nicotinamide and quinone coenzymes. Biochimica et Biophysica Acta (BBA)-General Subjects. 1995 Dec 14;1245(3):366-70.

Background

Ethyl 2-acetoxy-2-methylacetoacetate is a multifunctional β -ketoester derivative that has the chemical activity of ester, ketone and acetoxy. It is widely used in the synthesis of pharmaceutical intermediates and material monomers^[1]. Due to its high reactivity, it needs to be stored at low temperature and away from light, and protection should be taken during operation.

References:

- [1]. Xing RY, Whitman WB. Characterization of enzymes of the branched-chain amino acid biosynthetic pathway in Methanococcus spp. Journal of bacteriology. 1991 Mar;173(6):2086-92.

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