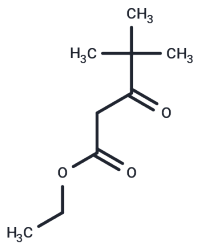
Data Sheet (Cat.No.T78505)

TargetMol

Ethyl pivaloylacetate

Chemical Properties



CAS No. : 17094-34-7

Formula: C9H16O3

Molecular Weight: 172.22

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	Ethyl pivaloylacetate is a significant β-ketoester. It is widely employed as a model substrate in biocatalysis to evaluate the catalytic activity and stereoselectivity of ketoreductase (KRED) tool-boxes. Due to the presence of the bulky pivaloyl (tert-butyl) group, it serves as an excellent probe for assessing the substrate pocket size and enantioselectivity of recombinant enzymes. The enzymatic reduction of this compound yields enantiopure β-hydroxyesters, which are essential chiral building blocks for the synthesis of sophisticated pharmaceutical intermediates.
Targets(IC50)	Others
In vitro	Ethyl pivaloylacetate serves as a standard substrate for ketoreductase (KRED) kinetics, with activity quantified by NADPH absorbance decay at 340 nm. It enables screening for sterically tolerant enzyme variants and profiling KRED stereopreferences, offering key data for biotransformation development [1].

Solubility Information

Solubility	DMSO: 80 mg/mL (464.52 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	5.8065 mL	29.0326 mL	58.0653 mL
5 mM	1.1613 mL	5.8065 mL	11.6131 mL
10 mM	0.5807 mL	2.9033 mL	5.8065 mL
50 mM	0.1161 mL	0.5807 mL	1.1613 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Zhu D, et, al. A recombinant ketoreductase tool-box. Assessing the substrate selectivity and stereoselectivity toward the reduction of β-ketoesters. Tetrahedron. 2006 Jan; 62 (5): 901-905.