



KALPASTHANA LIFE CARE PRODUCTS PVT. LTD.

Regd. Office: Plot No. 92P & 93, KIADB Industrial Area, Humnabad, Bidar District, Karnataka - 585330, India.

Email: info@kalpasthanalifecareproducts.com | Website: www.kalpasthanalifecareproducts.com

TECHNICAL DATA SHEET

Methyl 4-acetyl-5-oxohexanoate

CAS No: 13984-53-7

PRODUCT DESCRIPTION

A high-purity tri-carbonyl intermediate used as a key starting material (KSM) or building block for pyrrole synthesis (Knorr condensation) and biological drug discovery applications. This multifunctional compound contains a methyl ester, an acetyl group, and a ketone, offering unique reactivity profiles. Kalpasthana Life Care Products ensures strict quality testing and consistency to support advanced pharmaceutical and research applications.

SPECIFICATIONS

Product Name	Methyl 4-acetyl-5-oxohexanoate
Synonyms / Alternate Names	4-Acetyl-5-oxohexanoic acid methyl ester, Methyl 4-acetyl-5-oxohexanoate
CAS Number	13984-53-7
Molecular Formula	C ₉ H ₁₄ O ₄
Molecular Weight	186.21 g/mol
Appearance	Colorless to light yellow liquid or low-melting solid
Purity (GC)	≥ 98.0%
Boiling Point	110°C - 114°C at 5 mmHg

APPLICATIONS & USAGE

Methyl 4-acetyl-5-oxohexanoate is a highly functionalized tri-carbonyl intermediate widely utilized in heterocyclic chemistry and drug discovery. It is an essential building block for constructing substituted pyrrole rings via modified Knorr and Paal-Knorr condensations. It serves as a key structural scaffold for the synthesis of complex active pharmaceutical ingredients (APIs), including PD-1/PD-L1 pathway inhibitors and agricultural fungicides.

- Substituted Pyrroles: Essential reactant for synthesizing highly substituted pyrrole-3-carboxylic acid esters (structures related to Atorvastatin family).
- Biomedical Research: Acts as a key scaffold for constructing compound libraries in oncology, immunology, and receptor targeting.
- Agrochemical Intermediates: Precursor for synthesizing nitrogen-rich heterocyclic fungicides, insecticides, and crop protection agents.

DISCLAIMER & SAFETY

Disclaimer: The information contained in this Technical Data Sheet is accurate to the best of our knowledge. It is provided for informational purposes only. The user assumes all risk and liability for the product's use in manufacturing or commercial applications. Products are intended for industrial manufacturing and laboratory research purposes only. Please refer to the Material Safety Data Sheet (MSDS) for detailed safety, handling, storage, and disposal guidelines.