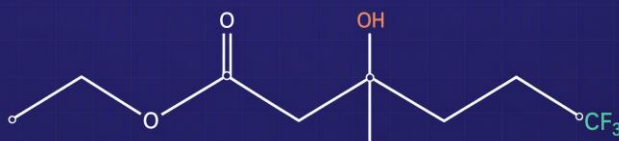


Ethyl 7,7,7-trifluoro-3-hydroxy-3-methylheptanoate



PRODUCT IN FOCUS



Ethyl 7,7,7-trifluoro-3-hydroxy-3-methylheptanoate

INTRODUCTION

Ethyl 7,7,7-trifluoro-3-hydroxy-3-methylheptanoate is a fluorinated aliphatic hydroxy ester. The presence of the trifluoromethyl group imparts enhanced metabolic stability, lipophilicity, and unique physicochemical properties compared with non-fluorinated analogues. This compound is primarily used as a synthetic intermediate in pharmaceutical and agrochemical research.

MANUFACTURE

Ethyl 7,7,7-trifluoro-3-hydroxy-3-methylheptanoate can be synthesized in a convenient three-step process starting from 4,4,4-trifluoro-1-butanol. Halogenation of 4,4,4-trifluoro-1-butanol affords 1-halo-4,4,4-trifluorobutane, which is converted into the corresponding Grignard reagent under standard reaction conditions. The resulting Grignard reagent is then reacted with *N*-methoxy-*N*-methylacetamide under carefully controlled conditions to furnish the desired ethyl 7,7,7-trifluoro-3-hydroxy-3-methylheptanoate.

APPLICATIONS

Ethyl 7,7,7-trifluoro-3-hydroxy-3-methylheptanoate is widely recognized as a research intermediate for fluorinated organic synthesis. The main areas of application include:

Pharmaceutical Industry:

- Used in the synthesis of fluorinated drug candidates.
- Serves as a building block for introducing CF₃-containing side chains into biologically active molecules.
- Useful in medicinal chemistry programs aimed at improving metabolic stability and pharmacokinetic properties.

Medicinal chemistry research:

- Provides a versatile scaffold containing both a hydroxyl and an ester functional group, allowing further transformations such as oxidation, esterification, reduction, amide formation, etc.

Fluorinated building block:

- Useful for structure–activity relationship (SAR) studies where incorporation of a trifluoromethyl group is desired.

Agrochemical research:

- Potential intermediate for synthesizing fluorinated herbicide, fungicide, or insecticide candidates, as fluorinated substituents are commonly used to improve chemical stability and biological activity.

Organic synthesis:

- Serves as a specialty intermediate in academic and industrial laboratories for developing new fluorinated molecules and fine chemicals.

Synonyms

Heptanoic acid, 7,7,7-trifluoro-3-hydroxy-3-methyl-, ethyl ester; 7,7,7-Trifluoro-3-hydroxy-3-methylheptanoic acid ethyl ester.

CAS no.

1602476-15-2

EINECS no.

N/A

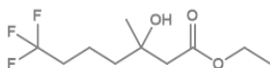
Molecular formula

C₁₀H₁₇F₃O₃

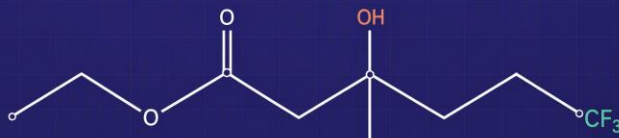
Molecular weight

242.24

Structure



Ethyl 7,7,7-trifluoro-3-hydroxy-3-methylheptanoate



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SPECIFICATIONS

Test	Unit	Specification
Identification by:		
• ¹ H NMR	-	Conform to the structure
• LCMS		<i>m/z</i> Complies with exact mass of the product
Purity (By GC)	%	Min 95.0

STORAGE & PRECAUTION

Store the container tightly closed in a dry, cool and well-ventilated place.

PACKING

UN Approved drums;

Packaging quantities: 30 kg/drum, 250 kg/drum

REACH Status

Not registered

ExSyn offers Ethyl 7,7,7-trifluoro-3-hydroxy-3-methylheptanoate on a commercial scale and welcomes your enquiries. Regardless of the quantity required, our commitment to exceptional quality and reliable service makes ExSyn the preferred supplier of choice! Should you require any additional information, please feel free to contact us.