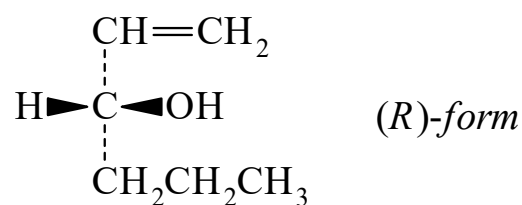




>>Entry Name: 1-Hexen-3-ol, 9CI
ENTRY UNDER REVIEW



CAS Registry Number: 4798-44-1

Molecular Formula: C₆H₁₂O
Molecular Weight: 100.16
Accurate Mass: 100.088815
Percentage Composition: C 71.95%; H 12.08%; O 15.97%
Biological Source: Constit. of the essential oils of various plant spp.
Use/Importance: Flavouring ingredient

Aldrich: W36080-5

>>Variant: (R)-form

Molecular Formula: C₆H₁₂O
Molecular Weight: 100.16
Accurate Mass: 100.088815
Percentage Composition: C 71.95%; H 12.08%; O 15.97%
Boiling Point: Bp₉₀ 70-72°
Optical Rotation: [α]_D -28.2. [α]_D²⁰ -14.7 (c, 1.9 in CHCl₃) (99% ee)

>>Derivative: Strychnine salt

Melting Point: Mp 170°

>>Derivative: Acid phthalate

Melting Point: Mp 62-63°

>>Variant: (±)-form

CAS Registry Number: 67928-93-2
Molecular Formula: C₆H₁₂O
Molecular Weight: 100.16
Accurate Mass: 100.088815
Percentage Composition: C 71.95%; H 12.08%; O 15.97%
Boiling Point: Bp 133.5-134°. Bp₂₀ 49-51°

>>Derivative: 4-Nitrobenzoyl
Synonym(s): FEMA 3352

Molecular Formula: C₁₃H₁₅NO₄
Molecular Weight: 249.266
Percentage Composition: C 62.64%; H 6.07%; N 5.62%; O 25.67%
Melting Point: Mp 60-62°

>>Derivative: Me ether
Synonym(s): 3-Methoxy-1-hexene

Molecular Formula: C₇H₁₄O
Molecular Weight: 114.187
Accurate Mass: 114.104465
Percentage Composition: C 73.63%; H 12.36%; O 14.01%
Physical Description: Liq.
Boiling Point: Bp 113-115° (88-91°)

References: