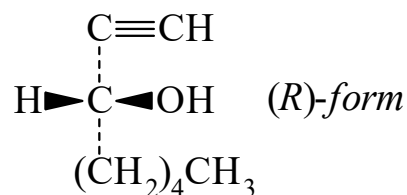




>>Entry Name: 1-Octyn-3-ol, 9CI



CAS Registry Number: 818-72-4

Molecular Formula: C₈H₁₄O

Molecular Weight: 126.198

Accurate Mass: 126.104465

Percentage Composition: C 76.14%; H 11.18%; O 12.68%

Aldrich: 12728-0

Fluka: 74973

>>Variant: (R)-form

CAS Registry Number: 32556-70-0

Molecular Formula: C₈H₁₄O

Molecular Weight: 126.198

Accurate Mass: 126.104465

Percentage Composition: C 76.14%; H 11.18%; O 12.68%

Use/Importance: Intermediate in prostaglandin synth.

Boiling Point: Bp₂₀ 100°

Optical Rotation: [α]_D²⁰ +14.9 (c, 1 in dioxan) (*ca.* 100% ee)

Aldrich: 39970-1

>>Variant: (S)-form

CAS Registry Number: 32556-71-1

Molecular Formula: C₈H₁₄O

Molecular Weight: 126.198

Accurate Mass: 126.104465

Percentage Composition: C 76.14%; H 11.18%; O 12.68%

Physical Description: Oil

Boiling Point: Bp₂₀ 88-89°

Optical Rotation: [α]_D²² -22.2 (c, 1.6 in Et₂O). [α]_D²⁰ -15.7 (c, 1 in dioxan) (*ca.* 100% ee)

Aldrich: 39396-7

>>Variant: (±)-form

Molecular Formula: C₈H₁₄O

Molecular Weight: 126.198

Accurate Mass: 126.104465

Percentage Composition: C 76.14%; H 11.18%; O 12.68%

Boiling Point: Bp₁₉ 83°

References:

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