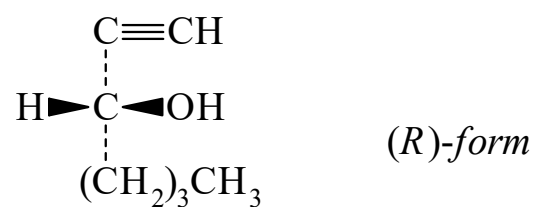




>>Entry Name: 1-Heptyn-3-ol, 9CI



CAS Registry Number: 7383-19-9

Related CAS Registry Numbers(s): 51586-58-4 51703-66-3

Molecular Formula: $C_7H_{12}O$

Molecular Weight: 112.171

Accurate Mass: 112.088815

Percentage Composition: C 74.95%; H 10.78%; O 14.26%

>>Variant: (R)-form

CAS Registry Number: 51703-65-2

Molecular Formula: $C_7H_{12}O$

Molecular Weight: 112.171

Accurate Mass: 112.088815

Percentage Composition: C 74.95%; H 10.78%; O 14.26%

Optical Rotation: $[\alpha]_D^{25} +20.5$ (c, 3.0 in dioxan) (100% ee)

>>Derivative: Me ether

Synonym(s): 3-Methoxy-1-heptyne

CAS Registry Number: 102276-17-5

Molecular Formula: $C_8H_{14}O$

Molecular Weight: 126.198

Accurate Mass: 126.104465

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

Physical Description: Liq.

Boiling Point: Bp 135°

Optical Rotation: $[\alpha]_D^{25} +55.4$ (c, 3.39 in Et₂O) (58% ee)

>>Derivative: Ac

CAS Registry Number: 65253-18-1

Molecular Formula: $C_9H_{14}O_2$

Molecular Weight: 154.208

Accurate Mass: 154.09938

Percentage Composition: C 70.10%; H 9.15%; O 20.75%

Optical Rotation: $[\alpha]_D^{25} +19.6$ (c, 2.1 in Et₂O) (28% ee)

>>Variant: (S)-form

CAS Registry Number: 51703-66-3

Molecular Formula: $C_7H_{12}O$

Molecular Weight: 112.171

Accurate Mass: 112.088815

Percentage Composition: C 74.95%; H 10.78%; O 14.26%

Optical Rotation: $[\alpha]_D^{25} -18.8$ (c, 5.2 in dioxan) (>98% ee). $[\alpha]_D^{25} -15$ (c, 2.6 in dioxan)

>>Variant: (±)-form

CAS Registry Number: 51586-58-4

Molecular Formula: $C_7H_{12}O$

Molecular Weight: 112.171

Accurate Mass: 112.088815

Percentage Composition: C 74.95%; H 10.78%; O 14.26%

Physical Description: Liq.

Boiling Point: Bp₁₈ 67-69°. Bp₅ 55-60°

Density: d₂₀ 0.87

References: