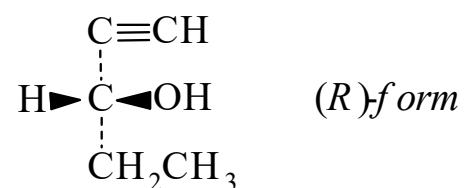




>>Entry Name: 1-Pentyn-3-ol, 9CI

Synonym(s): Ethylethynylcarbinol. 3-Hydroxy-1-pentyne



CAS Registry Number: 4187-86-4

Molecular Formula: C₅H₈O

Molecular Weight: 84.118

Accurate Mass: 84.057515

Percentage Composition: C 71.39%; H 9.59%; O 19.02%

Aldrich: E2840-4

>>Variant: (R)-form

Molecular Formula: C₅H₈O

Molecular Weight: 84.118

Accurate Mass: 84.057515

Percentage Composition: C 71.39%; H 9.59%; O 19.02%

Physical Description: Liq.

Optical Rotation: $[\alpha]_{\text{Hg}}^{20} +36.8$ (c, 2.5 in Et₂O)

>>Derivative: 2-Carboxy-3-nitrobenzoyl

Physical Description: Cryst.

Melting Point: Mp 136°

Optical Rotation: $[\alpha]_{\text{Hg}}^{20} -0.4$ (c, 2.5 in MeOH)

>>Variant: (±)-form

Molecular Formula: C₅H₈O

Molecular Weight: 84.118

Accurate Mass: 84.057515

Percentage Composition: C 71.39%; H 9.59%; O 19.02%

Boiling Point: Bp 125°

>>Derivative: 3,5-Dinitrobenzoyl

Physical Description: Needles (EtOH)

Melting Point: Mp 91°

References:

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McGrew, F.C. *et al.*, *J.A.C.S.*, 1937, **59**, 1497, (*synth*)

Bohlmann, F. *et al.*, *Chem. Ber.*, 1965, **98**, 2608, (*resoln, abs config*)

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