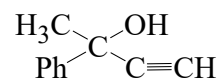




>>Entry Name: 2-Phenyl-3-butyn-2-ol

Synonym(s): α -Ethynyl- α -methylbenzenemethanol, 9CI



CAS Registry Number: 127-66-2

Molecular Formula: C₁₀H₁₀O

Molecular Weight: 146.188

Accurate Mass: 146.073165

Percentage Composition: C 82.16%; H 6.89%; O 10.94%

Use/Importance: Hypnotic

Aldrich: 21299-7

Fluka: 78230

Rare Chemicals Library: S35115-6

Sigma: P0522

>>Variant: ($\pm$)-form

Molecular Formula: C₁₀H₁₀O

Molecular Weight: 146.188

Accurate Mass: 146.073165

Percentage Composition: C 82.16%; H 6.89%; O 10.94%

Melting Point: Mp 49°

Boiling Point: Bp₄ 82-83°

>>Derivative: Ac

CAS Registry Number: 15963-07-2

Molecular Formula: C₁₂H₁₂O₂

Molecular Weight: 188.226

Accurate Mass: 188.08373

Percentage Composition: C 76.57%; H 6.43%; O 17.00%

Physical Description: Viscous liq.

Boiling Point: Bp₉ 112-113°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 535B, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 947B, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1599C, (*ir*)

Papa, D. *et al.*, *J.A.C.S.*, 1954, **76**, 4446, (*synth*)

Nazarov, I.N. *et al.*, *CA*, 1955, **49**, 927, (*synth*)

Kriz, J. *et al.*, *Coll. Czech. Chem. Comm.*, 1967, **32**, 398, (*synth*)

Hearn, M.T.W., *Tetrahedron*, 1976, **32**, 115, (*cmr*)