



>>Entry Name: 2-Methyl-3-butyn-2-ol, 9CI

Synonym(s): Ethynyldimethylcarbinol

CAS Registry Number: 115-19-5

$(\text{H}_3\text{C})_2\text{C}(\text{OH})\text{C}\equiv\text{CH}$

Molecular Formula: $\text{C}_5\text{H}_8\text{O}$

Molecular Weight: 84.118

Accurate Mass: 84.057515

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

Use/Importance: Intermed. in the manuf. of terpene alcohols for the perfumery industry and in the manuf. of isoprene

Physical Description: Liq.

Melting Point: Fp 2.6°

Boiling Point: Bp $104\text{--}106^\circ$. Bp₁₂ 20°

Solubility: Misc. H_2O ; sol. most org. solvs.

Density: d_4^{20} 0.862

Refractive Index: n_D^{20} 1.4207

Other Data: Forms azeotrope containing 26% H_2O , Bp 90° . Undergoes Pd-catalysed homopolym.

Hazard & Toxicity: LD₅₀ (rat, orl) 1950 mg/kg

Aldrich: 12976-3

Fluka: 66120

>>Derivative: Ac

CAS Registry Number: 1604-29-1

Molecular Formula: $\text{C}_7\text{H}_{10}\text{O}_2$

Molecular Weight: 126.155

Accurate Mass: 126.06808

Percentage Composition: C 66.65%; H 7.99%; O 25.36%

Boiling Point: Bp 131° . Bp₁₅ $38\text{--}40^\circ$

Rare Chemicals Library: S30320-8

>>Derivative: Me ether

Synonym(s): 3-Methoxy-3-methyl-1-butyne

CAS Registry Number: 13994-57-5

Molecular Formula: $\text{C}_6\text{H}_{10}\text{O}$

Molecular Weight: 98.144

Accurate Mass: 98.073165

Percentage Composition: C 73.43%; H 10.27%; O 16.30%

Boiling Point: Bp 78.5°

Hazard & Toxicity: Highly flammable, fl. p. $<21^\circ$

References:

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