



>>Entry Name: 2,2-Dimethyl-1-propanol

Synonym(s): *tert*-Butylcarbinol. Neopentyl alcohol. Neoamyl alcohol

CAS Registry Number: 75-84-3

(H₃C)₃CCH₂OH

Molecular Formula: C₅H₁₂O

Molecular Weight: 88.149

Accurate Mass: 88.088815

Percentage Composition: C 68.13%; H 13.72%; O 18.15%

Physical Description: Cryst.

Melting Point: Mp 52-53°

Boiling Point: Bp 113°

Hazard & Toxicity: Flammable, fl. p. 37°, autoignition temp. 225°

Aldrich: N720-6

Fluka: 41520

>>Derivative: Ac

CAS Registry Number: 926-41-0

Molecular Formula: C₇H₁₄O₂

Molecular Weight: 130.186

Accurate Mass: 130.09938

Percentage Composition: C 64.58%; H 10.84%; O 24.58%

Physical Description: Liq.

Boiling Point: Bp 125.5-126°

>>Derivative: 4-Methylbenzenesulfonyl

CAS Registry Number: 2346-07-8

Physical Description: Cryst. (MeOH aq. or hexane/C₆H₆)

Melting Point: Mp 47-48° (44-45°)

Rare Chemicals Library: S77907-5

>>Derivative: Me ether

Synonym(s): 1-Methoxy-2,2-dimethylpropane, 9Cl. Methyl neopentyl ether

CAS Registry Number: 1118-00-9

Molecular Formula: C₆H₁₄O

Molecular Weight: 102.176

Accurate Mass: 102.104465

Percentage Composition: C 70.53%; H 13.81%; O 15.66%

Physical Description: Liq.

Boiling Point: Bp 80-81°

>>Derivative: Et ether

Synonym(s): 1-Ethoxy-2,2-dimethylpropane, 9Cl. Ethyl neopentyl ether

CAS Registry Number: 17348-57-1

Molecular Formula: C₇H₁₆O

Molecular Weight: 116.203

Accurate Mass: 116.120115

Percentage Composition: C 72.35%; H 13.88%; O 13.77%

Physical Description: Liq.

Boiling Point: Bp 91.5°

References:

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Samec, M., *Annalen*, 1907, **351**, 255, (*synth*)
Merz, A., *Angew. Chem., Int. Ed.*, 1973, **12**, 846, (*Me ether*)
Bowen, R.D. *et al.*, *J.C.S. Perkin 2*, 1984, 1005, (*ms*)
Chauvel, J.P. *et al.*, *Chem. Phys.*, 1985, **95**, 435, (*pmr*)
Reuben, J., *J.A.C.S.*, 1985, **107**, 1756, (*cmr*)
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