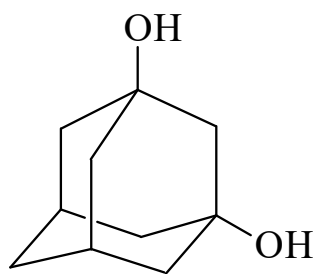




>>Entry Name: 1,3-Adamantanediol

Synonym(s): Tricyclo[3.3.1.1^{3,7}]decane-1,3-diol, 9CI



CAS Registry Number: 5001-18-3

Molecular Formula: C₁₀H₁₆O₂

Molecular Weight: 168.235

Accurate Mass: 168.11503

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

Physical Description: Cryst. (MeOH/hexane or CHCl₃)

Melting Point: Mp 256-258°. Mp 315°

Rare Chemicals Library: S94686-9

>>Derivative: Di-Ac

CAS Registry Number: 29817-47-8

Molecular Formula: C₁₄H₂₀O₄

Molecular Weight: 252.31

Accurate Mass: 252.13616

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

Physical Description: Oil

>>Derivative: Mono-Me ether

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

Molecular Formula: C₁₁H₁₈O₂

Molecular Weight: 182.262

Accurate Mass: 182.13068

Percentage Composition: C 72.49%; H 9.95%; O 17.56%

Physical Description: Needles (petrol)

Melting Point: Mp 64-65°

>>Derivative: Mono-Et ether

Synonym(s): 3-Ethoxy-1-adamantanol

CAS Registry Number: 1078-86-0

Molecular Formula: C₁₂H₂₀O₂

Molecular Weight: 196.289

Accurate Mass: 196.14633

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

Physical Description: Plates (petrol)

Melting Point: Mp 77.5°

References:

- Stetter, H. *et al.*, *Chem. Ber.*, 1960, **93**, 1366; 1965, **98**, 3888, (*O-Et synth*)
Lunn, W.H.W., *J.C.S.(C)*, 1970, 2124, (*Di-Ac synth, pmr*)
Fischer, W. *et al.*, *Helv. Chim. Acta*, 1976, **59**, 1953, (*OMe synth, ir, pmr*)
Fischer, W. *et al.*, *Helv. Chim. Acta*, 1978, **61**, 1588, (*synth*)
Mello, R. *et al.*, *J.A.C.S.*, 1989, **111**, 6749, (*synth, ir, pmr, ms*)
Murray, R.W. *et al.*, *J.O.C.*, 1995, **60**, 5673, (*synth, cmr, pmr, ir*)
Muraoka, O. *et al.*, *Synth. Commun.*, 1996, **26**, 1555, (*synth*)