



>>Entry Name: 2-Hydroxymethyl-1,3-propanediol, 9CI

Synonym(s): Tris(hydroxymethyl)methane

CAS Registry Number: 4704-94-3

CH(CH₂OH)₃

Molecular Formula: C₄H₁₀O₃

Molecular Weight: 106.121

Accurate Mass: 106.062995

Percentage Composition: C 45.27%; H 9.50%; O 45.23%

Physical Description: Chunky prisms (Me₂CO)

Melting Point: Mp 67-68° (60-63°)

Boiling Point: Bp_{2.5} 130-135° subl.

Aldrich: 39365-7

Fluka: 55762

>>Derivative: Tribenzoyl

CAS Registry Number: 113967-50-3

Molecular Formula: C₂₅H₂₂O₆

Molecular Weight: 418.445

Accurate Mass: 418.14164

Percentage Composition: C 71.76%; H 5.30%; O 22.94%

Physical Description: Needles (hexane)

Melting Point: Mp 75-76°

>>Derivative: Tris(methanesulfonyl)

CAS Registry Number: 113967-52-5

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 83-84°

>>Derivative: Mono-Et ether

Synonym(s): 2-(Ethoxymethyl)-1,3-propanediol

Molecular Formula: C₆H₁₄O₃

Molecular Weight: 134.175

Accurate Mass: 134.094295

Percentage Composition: C 53.71%; H 10.52%; O 35.77%

Physical Description: Oil

Boiling Point: Bp_{0.5} 84-88°

References:

Dekmizian, A.H. *et al.*, *Synth. Commun.*, 1979, **9**, 431, (*synth, ir, pmr*)

Nielsen, A.T. *et al.*, *Pol. J. Chem. (Rocz. Chem.)*, 1981, **55**, 1393, (*synth, pmr, cmr*)

Latour, S. *et al.*, *Synthesis*, 1987, 742, (*synth, ms, ir, pmr*)

Harnden, M.R. *et al.*, *J. Med. Chem.*, 1990, **33**, 187, (*synth, ir, pmr*)

Childs, R.F. *et al.*, *Can. J. Chem.*, 1994, **72**, 2084, (*mono-Et ether, synth, pmr*)