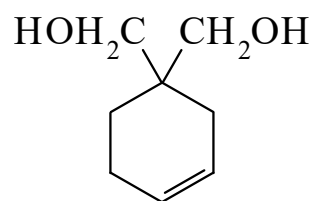




>>Entry Name: 3-Cyclohexene-1,1-dimethanol, 9CI

Synonym(s): 4,4-Bis(hydroxymethyl)cyclohexene



CAS Registry Number: 2160-94-3

Related CAS Registry Numbers(s): 66810-09-1

Molecular Formula: C₈H₁₄O₂

Molecular Weight: 142.197

Accurate Mass: 142.09938

Percentage Composition: C 67.57%; H 9.92%; O 22.50%

Aldrich: 16215-9

Fluka: 14915

>>Variant: (±)-form

Molecular Formula: C₈H₁₄O₂

Molecular Weight: 142.197

Accurate Mass: 142.09938

Percentage Composition: C 67.57%; H 9.92%; O 22.50%

Use/Importance: Used for cross-linking epoxy resins and in other polymers

Physical Description: Cryst. (Me₂CO aq.)

Melting Point: Mp 94.5-95° (87°)

Boiling Point: Bp₃ 128°

>>Derivative: Di-Ac

CAS Registry Number: 27025-19-0

Molecular Formula: C₁₂H₁₈O₄

Molecular Weight: 226.272

Accurate Mass: 226.12051

Percentage Composition: C 63.70%; H 8.02%; O 28.28%

Physical Description: Oil

Refractive Index: n_D²⁵ 1.4646

>>Derivative: Bis(4-methylbenzenesulfonyl)

Physical Description: Solid

Melting Point: Mp 75.5-76.5°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 261B, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 166C, (*ir*)

Campbell, T.W. *et al.*, *J.O.C.*, 1961, **26**, 4654, (*synth*)

Grubbs, E.J. *et al.*, *J.O.C.*, 1971, **36**, 504, (*synth*, *pmr*, *ir*)