



>>Entry Name: **2-(Hydroxymethyl)-2-methyl-1,3-propanediol**, 9CI

Synonym(s): 1,1,1-Tris(hydroxymethyl)ethane. Pentaglycerol. Metriol. Trimethylolethane. Ethylidynetrimethanol. TME

CAS Registry Number: 77-85-0

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

Molecular Formula: $\text{C}_5\text{H}_{12}\text{O}_3$

Molecular Weight: 120.148

Accurate Mass: 120.078645

Percentage Composition: C 49.98%; H 10.07%; O 39.95%

Source/Synthesis: Obt. industrially by reacn. of 1-Propanol [DFP00-K](#) with Formaldehyde [CVP49-C](#)

Use/Importance: Monomer used in alkyd resins for paints. Intermed. for industrial chemicals and explosives

Melting Point: Mp 202-203°

Boiling Point: Bp_{0.1} 150°

Solubility: Sol. H_2O , EtOH

Other Data: Sublimes

Aldrich: T8780-7

Fluka: 93340

Sigma: H5030

>>Derivative: Tri-Ac

CAS Registry Number: 13431-59-9

Molecular Formula: $\text{C}_{11}\text{H}_{18}\text{O}_6$

Molecular Weight: 246.26

Accurate Mass: 246.11034

Percentage Composition: C 53.65%; H 7.37%; O 38.98%

Boiling Point: Bp₁₅ 161-162°

Rare Chemicals Library: S41175-2

>>Derivative: Tris(4-methylbenzenesulfonyl)

Physical Description: Needles

Melting Point: Mp 108-108.5°

>>Derivative: Tris(3-mercaptopropanoyl)

CAS Registry Number: 10312-58-0

Molecular Formula: $\text{C}_{14}\text{H}_{24}\text{O}_6\text{S}_3$

Molecular Weight: 384.538

Accurate Mass: 384.0735

Percentage Composition: C 43.73%; H 6.29%; O 24.96%; S 25.02%

Use/Importance: Cross-linking agent for polymers

Boiling Point: Bp₁ 240°

Rare Chemicals Library: S51114-5

Other: PB T28415

>>Derivative: *O*-Isopropylidene

Synonym(s): 2,2,5-Trimethyl-1,3-dioxane-5-methanol, 9CI

CAS Registry Number: 3663-46-5

Molecular Formula: $\text{C}_8\text{H}_{16}\text{O}_3$

Molecular Weight: 160.213

Accurate Mass: 160.109945

Percentage Composition: C 59.98%; H 10.07%; O 29.96%

Physical Description: Oil

>>Derivative: Monobenzyl ether

CAS Registry Number: 4270-73-9

Molecular Formula: $\text{C}_{12}\text{H}_{18}\text{O}_3$

Molecular Weight: 210.272

Accurate Mass: 210.125595

Percentage Composition: C 68.55%; H 8.63%; O 22.83%

Physical Description: Cryst. (toluene/hexane)

Melting Point: Mp 44-45°