



>>Entry Name: 4-(Hydroxymethyl)benzoic acid, 9CI

Synonym(s): α -Hydroxy-*p*-toluic acid, 8CI. Benzyl alcohol 4-carboxylic acid. 4-Carboxybenzyl alcohol

CAS Registry Number: 58590-49-1

Related CAS Registry Numbers(s): 3006-96-0

Molecular Formula: C₈H₈O₃

Molecular Weight: 152.149

Accurate Mass: 152.047345

Percentage Composition: C 63.15%; H 5.30%; O 31.55%

Physical Description: Plates or needles (H₂O), needles by subl.

Melting Point: Mp 183°

>>Derivative: Et ester

CAS Registry Number: 15852-63-8

Molecular Formula: C₁₀H₁₂O₃

Molecular Weight: 180.203

Accurate Mass: 180.078645

Percentage Composition: C 66.65%; H 6.71%; O 26.64%

Boiling Point: Bp₅ 161-163°

>>Derivative: Nitrile

Synonym(s): 4-Cyanobenzyl alcohol

CAS Registry Number: 874-89-5

Molecular Formula: C₈H₇NO

Molecular Weight: 133.149

Accurate Mass: 133.052764

Percentage Composition: C 72.17%; H 5.30%; N 10.52%; O 12.02%

Physical Description: Leaflets (EtOAc)

Melting Point: Mp 133-134°

>>Derivative: Benzoyl

Molecular Formula: C₁₅H₁₂O₄

Molecular Weight: 256.257

Accurate Mass: 256.07356

Percentage Composition: C 70.31%; H 4.72%; O 24.97%

Physical Description: Oil

Boiling Point: Bp₃ 203-207°

>>Derivative: Me ether

Synonym(s): 4-(Methoxymethyl)benzoic acid

CAS Registry Number: 6908-41-4

Molecular Formula: C₉H₁₀O₃

Molecular Weight: 166.176

Accurate Mass: 166.062995

Percentage Composition: C 65.05%; H 6.07%; O 28.88%

Physical Description: Leaflets (H₂O)

Melting Point: Mp 123°

Aldrich: 26647-7

>>Derivative: Et ether

Synonym(s): 4-(Ethoxymethyl)benzoic acid

Molecular Formula: C₁₀H₁₂O₃

Molecular Weight: 180.203

Accurate Mass: 180.078645

Percentage Composition: C 66.65%; H 6.71%; O 26.64%

Physical Description: Plates (H₂O)

Melting Point: Mp 87°

References: