



>>Entry Name: 4-Hydroxybutanoic acid, 9CI

CAS Registry Number: 591-81-1

Related CAS Registry Numbers(s): 35054-79-6

Extra CAS Registry Numbers(s): 114-63-6

HOH₂C(CH₂)₂COOH

Molecular Formula: C₄H₈O₃

Molecular Weight: 104.105

Accurate Mass: 104.047345

Percentage Composition: C 46.15%; H 7.75%; O 46.11%

Physical Description: Liq. at -17°

pKa Value: pK_a 4.71

Calculated Log P Data: Log P -1.16 (calc)

Other Data: Lactonises above -17°

>>Derivative: Na salt

Synonym(s): Sodium oxybate. Anetamin. Gamanest. Gioron. Oxybate sodium. Somsanit. NSC 84223. WY 3478

CAS Registry Number: 502-85-2

Biological Use/Importance: Adjunct to anaesthesia. Hypnotic. Putative neurotransmitter, low oral toxicity

Physical Description: Cryst. (EtOH)

Melting Point: Mp 145-146°

Aldrich: H2222-1

Fluka: 54970

Sigma: H4517

>>Derivative: Me ester

CAS Registry Number: 925-57-5

Molecular Formula: C₅H₁₀O₃

Molecular Weight: 118.132

Accurate Mass: 118.062995

Percentage Composition: C 50.84%; H 8.53%; O 40.63%

Boiling Point: Bp_{0.5} 45°

>>Derivative: Et ester

CAS Registry Number: 999-10-0

Molecular Formula: C₆H₁₂O₃

Molecular Weight: 132.159

Accurate Mass: 132.078645

Percentage Composition: C 54.53%; H 9.15%; O 36.32%

Boiling Point: Bp_{0.4} 57-58°. Bp₁₅ 99-103°

>>Derivative: Isopropyl ester

Molecular Formula: C₇H₁₄O₃

Molecular Weight: 146.186

Accurate Mass: 146.094295

Percentage Composition: C 57.51%; H 9.65%; O 32.83%

Boiling Point: Bp_{0.4} 64°

>>Derivative: Ac

Synonym(s): 4-Acetoxybutanoic acid. Aceburic acid, INN

CAS Registry Number: 26976-72-7

Molecular Formula: C₆H₁₀O₄

Molecular Weight: 146.143

Accurate Mass: 146.05791

Percentage Composition: C 49.31%; H 6.90%; O 43.79%

Biological Use/Importance: Analgesic

Boiling Point: Bp_{0.1} 102°

Solubility: Sol. H₂O