



>>Entry Name: 2-Hydroxy-2-methylpropanoic acid, 9CI

ENTRY UNDER REVIEW

Synonym(s): 2-Methylactic acid, 8CI. 2-Hydroxyisobutyric acid. Acetonic acid

CAS Registry Number: 594-61-6

$(\text{H}_3\text{C})_2\text{C}(\text{OH})\text{COOH}$

Molecular Formula: $\text{C}_4\text{H}_8\text{O}_3$

Molecular Weight: 104.105

Accurate Mass: 104.047345

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

Physical Description: Hygroscopic prisms (Et_2O)

Melting Point: Mp 79°

Boiling Point: Bp 212°. Bp₁₂ 114°

Solubility: Sol. H_2O ; spar. sol. C_6H_6

Aldrich: 16497-6

Fluka: 55390

Sigma: H9126

>>Derivative: Me ester

CAS Registry Number: 2110-78-3

Molecular Formula: $\text{C}_5\text{H}_{10}\text{O}_3$

Molecular Weight: 118.132

Accurate Mass: 118.062995

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

Physical Description: Oil

Boiling Point: Bp 137°

Aldrich: M5020-6

Fluka: 55410

>>Derivative: *tert*-Butyl ester

CAS Registry Number: 36293-63-7

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%

Refractive Index: n_{D}^{20} 1.4040

Aldrich: 38234-5

Fluka: 55405

>>Derivative: Amide

CAS Registry Number: 13027-88-8

Molecular Formula: $\text{C}_4\text{H}_9\text{NO}_2$

Molecular Weight: 103.121

Accurate Mass: 103.063329

Percentage Composition: C 46.59%; H 8.80%; N 13.58%; O 31.03%

Melting Point: Mp 98°

Boiling Point: Bp 260°

Solubility: V. sol. H_2O

>>Derivative: Nitrile

Synonym(s): 2-Hydroxy-2-methylpropanenitrile. 2-Cyano-2-propanol. 2-Hydroxyisobutyronitrile. Acetone cyanohydrin

CAS Registry Number: 75-86-5

Use/Importance: Used in place of HCN in Gattermann reaction for formylation of arenes

Melting Point: Mp -19°

Boiling Point: Bp₂₃ 82°

Solubility: V. sol. H_2O ; spar. sol. petrol

Hazard & Toxicity: Hydrolyses readily to HCN and Me_2CO . Fl. p. 64/74°, autoignition temp. 688°. LD₅₀ (rat, orl) 17.8 mg/kg. LD₅₀ (rbt, skn) 17 mg/kg. Human fatalities reported from skin contact or oral ingestion

Aldrich: A1000-0

Fluka: 591