



>>Entry Name: 3-Hydroxy-3-methylbutanoic acid, 9CI

Synonym(s): 3-Hydroxy-3-methylbutyric acid, 8CI. 3-Hydroxyisovaleric acid

CAS Registry Number: 625-08-1

Related CAS Registry Numbers(s): 18267-36-2

(H₃C)₂C(OH)CH₂COOH

Molecular Formula: C₅H₁₀O₃

Molecular Weight: 118.132

Accurate Mass: 118.062995

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

Physical Description: Oil

Boiling Point: Bp₁₂ 162°

Solubility: Sol. H₂O

pKa Value: pK_a 4.43

Fluka: 55453

>>Derivative: Me ester

CAS Registry Number: 6149-45-7

Molecular Formula: C₆H₁₂O₃

Molecular Weight: 132.159

Accurate Mass: 132.078645

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

Physical Description: Oil

Boiling Point: Bp₁₀ 70-71°

>>Derivative: Nitrile

Synonym(s): 1-Cyano-2-methyl-2-propanol

CAS Registry Number: 13635-04-6

Molecular Formula: C₅H₉NO

Molecular Weight: 99.132

Accurate Mass: 99.068414

Percentage Composition: C 60.58%; H 9.15%; N 14.13%; O 16.14%

Physical Description: Oil

Melting Point: Mp -12°

Boiling Point: Bp 210-212°. Bp₃₀ 130-132°

Solubility: Spar. sol. H₂O

Fluka: 55624

>>Derivative: Nitrile, O-β-D-glucopyranoside

Synonym(s): Epidermin‡

CAS Registry Number: 126050-09-7

Molecular Formula: C₁₁H₁₉NO₆

Molecular Weight: 261.274

Accurate Mass: 261.121239

Percentage Composition: C 50.57%; H 7.33%; N 5.36%; O 36.74%

Biological Source: Constit. of barley (*Hordeum vulgare*) and *Rhodotypos scandens*

>>Derivative: Ac, nitrile

Molecular Formula: C₇H₁₁NO₂

Molecular Weight: 141.169

Accurate Mass: 141.078979

Percentage Composition: C 59.56%; H 7.85%; N 9.92%; O 22.67%

Physical Description: Oil

Boiling Point: Bp 198-200°

>>Derivative: Phenylurethane

Melting Point: Mp 129-130°

References: