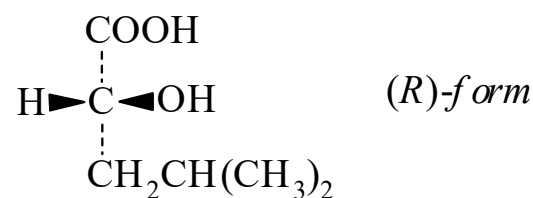




>>Entry Name: 2-Hydroxy-4-methylpentanoic acid, 9CI

ENTRY UNDER REVIEW

Synonym(s): 2-Hydroxy-4-methylvaleric acid, 8CI. Leucic acid. Leucinic acid



CAS Registry Number: 498-36-2

Molecular Formula: C₆H₁₂O₃

Molecular Weight: 132.159

Accurate Mass: 132.078645

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

Biological Source: Isol. from tobacco (*Nicotiana tabacum*)

Aldrich: 21981-9

>>Variant: (R)-form

CAS Registry Number: 20312-37-2

Molecular Formula: C₆H₁₂O₃

Molecular Weight: 132.159

Accurate Mass: 132.078645

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

Melting Point: Mp 80-81°

Optical Rotation: $[\alpha]_{\text{D}}^{22} +26.5$ (c, 1.52 in 1N NaOH)

>>Variant: (S)-form

CAS Registry Number: 13748-90-8

Molecular Formula: C₆H₁₂O₃

Molecular Weight: 132.159

Accurate Mass: 132.078645

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

Melting Point: Mp 80-81°

Optical Rotation: $[\alpha]_{\text{D}}^{22} -26.9$ (c, 1.55 in 1N NaOH)

Aldrich: 21982-7

Sigma: H9376

>>Derivative: Ac

CAS Registry Number: 3069-50-9

Molecular Formula: C₈H₁₄O₄

Molecular Weight: 174.196

Accurate Mass: 174.08921

Percentage Composition: C 55.16%; H 8.10%; O 36.74%

Physical Description: Oil

Boiling Point: Bp₂₀ 155-157°

>>Derivative: Ac, Me ester

Molecular Formula: C₉H₁₆O₄

Molecular Weight: 188.223

Accurate Mass: 188.10486

Percentage Composition: C 57.43%; H 8.57%; O 34.00%

Physical Description: Oil

Boiling Point: Bp₂₀ 103-104°

>>Derivative: Et ester

CAS Registry Number: 60856-85-1

Molecular Formula: C₈H₁₆O₃

Molecular Weight: 160.213

Accurate Mass: 160.109945

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

Boiling Point: Bp₁₂ 79-80°

Optical Rotation: $[\alpha]$