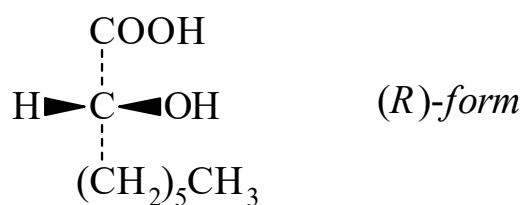




>>Entry Name: 2-Hydroxyoctanoic acid, 9CI, 8CI

Synonym(s): α -Hydroxycaprylic acid



CAS Registry Number: 617-73-2

Related CAS Registry Numbers(s): 6482-96-8

Molecular Formula: C₈H₁₆O₃

Molecular Weight: 160.213

Accurate Mass: 160.109945

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

Fluka: 56060

Rare Chemicals Library: S57684-0

Sigma: H7396

>>Variant: (R)-form

CAS Registry Number: 30117-44-3

Molecular Formula: C₈H₁₆O₃

Molecular Weight: 160.213

Accurate Mass: 160.109945

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

Physical Description: Cryst.

>>Derivative: Ba salt

Optical Rotation: $[\alpha]_{\text{D}}^{26} +9.1$ (1M NaOH)

>>Derivative: Me ester

CAS Registry Number: 92572-96-8

Molecular Formula: C₉H₁₈O₃

Molecular Weight: 174.239

Accurate Mass: 174.125595

Percentage Composition: C 62.04%; H 10.41%; O 27.55%

Physical Description: Liq.

Boiling Point: Bp₁₀ 110°

Optical Rotation: $[\alpha]_{\text{D}}^{20} -9.91$ (c, 1.95 in CHCl₃)

>>Derivative: *tert*-Butyl ester

Molecular Formula: C₁₂H₂₄O₃

Molecular Weight: 216.32

Accurate Mass: 216.172545

Percentage Composition: C 66.63%; H 11.18%; O 22.19%

Use/Importance: Chiral building block

Optical Rotation: $[\alpha]_{\text{D}}^{20} +3.7$ (c, 2 in CCl₄)

>>Variant: (S)-form

CAS Registry Number: 70267-27-5

Molecular Formula: C₈H₁₆O₃

Molecular Weight: 160.213

Accurate Mass: 160.109945

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

Physical Description: Cryst. (diisopropyl ether)

Melting Point: Mp 70.2-70.6°

Optical Rotation: $[\alpha]_{\text{D}}^{19} +6.2$ (c, 9 in CHCl₃)

>>Derivative: Ba salt

Physical Description: Cryst.

Optical Rotation: $[\alpha]_{\text{D}}^{26} -9.3$ (c, 1 in aq. NaCl)