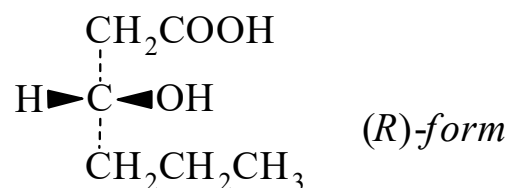




>>Entry Name: 3-Hydroxyhexanoic acid, 9CI, 8CI

ENTRY UNDER REVIEW

Synonym(s): 3-Hydroxycaproic acid



CAS Registry Number: 10191-24-9

Related CAS Registry Numbers(s): 66997-60-2

Molecular Formula: C₆H₁₂O₃

Molecular Weight: 132.159

Accurate Mass: 132.078645

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

>>Variant: (R)-form

CAS Registry Number: 77877-35-1

Molecular Formula: C₆H₁₂O₃

Molecular Weight: 132.159

Accurate Mass: 132.078645

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

Physical Description: Cryst. (petrol)

Melting Point: Mp 41-41.6°

Optical Rotation: $[\alpha]_D^{24}$ -27.9 (CHCl₃)

>>Derivative: Me ester

Molecular Formula: C₇H₁₄O₃

Molecular Weight: 146.186

Accurate Mass: 146.094295

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

Optical Rotation: $[\alpha]_D$ -27.1 (CHCl₃)

>>Variant: (±)-form

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 13°

Solubility: V. sol. H₂O

>>Derivative: Et ester

Synonym(s): FEMA 3545

CAS Registry Number: 2305-25-1

Molecular Formula: C₈H₁₆O₃

Molecular Weight: 160.213

Accurate Mass: 160.109945

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

Biological Source: Found in various fruits, presumably in an enantiomeric form

Use/Importance: Food flavourant

Physical Description: Liq. with fruity odour

Boiling Point: Bp₁₂ 95-98°

Aldrich: W35450-3

References:

Baker, C.F. *et al.*, *Annalen*, 1894, **283**, 124, (*synth*)

Lemieux, R.U. *et al.*, *Can. J. Chem.*, 1951, **29**, 678, (*abs config*)

Serck-Hanssen, K., *Ark. Kemi*, 1956, **10**, 136, (*abs config*)

Vuitel, L. *et al.*, *Helv. Chim. Acta*, 1974, **57**, 1713, (*nmr*)

Ketelaar, P.E.F. *et al.*, *Tet. Lett.*, 1985, **26**, 4665, (*synth*)

Burk, M.J. *et al.*, *J.A.C.S.*, 1993, **115**, 10125, (*synth, pmr*)

Yan, T.-H. *et al.*, *J.O.C.*, 1994, **59**, 8187; 1995, **60**, 3301, (*synth, ir, pmr, cmr*)