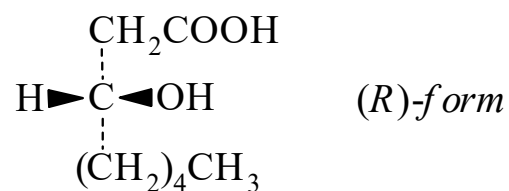




>>Entry Name: 3-Hydroxyoctanoic acid, 9CI

ENTRY UNDER REVIEW

Synonym(s): 3-Hydroxycaprylic acid



CAS Registry Number: 14292-27-4

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%

>>Variant: (R)-form

CAS Registry Number: 44987-72-6

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%

Biological Source: Isol. from secretion of the metathoracic glands of myrmicine ants. Also found in milk, strawberries and pineapple concentrate

Optical Rotation: $[\alpha]_{\text{D}}^{24} -21$ (c, 1.9 in CHCl_3)

>>Derivative: Me ester

CAS Registry Number: 78672-90-9

Molecular Formula: $\text{C}_9\text{H}_{18}\text{O}_3$

Molecular Weight: 174.239

Accurate Mass: 174.125595

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

Optical Rotation: $[\alpha]_{\text{D}}^{24} -18.4$ (c, 1 in CHCl_3)

>>Derivative: Hydrazide

Molecular Formula: $\text{C}_8\text{H}_{18}\text{N}_2\text{O}_2$

Molecular Weight: 174.242

Accurate Mass: 174.136828

Percentage Composition: C 55.15%; H 10.41%; N 16.08%; O 18.36%

Melting Point: Mp 127.5-128°

Optical Rotation: $[\alpha]_{\text{D}}^{24} -11.4$ (c, 1 in H_2O)

>>Variant: (S)-form

CAS Registry Number: 33796-86-0

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%

Melting Point: Mp 20-22°

Boiling Point: Bp_{0.15} 123°

Optical Rotation: $[\alpha]_{\text{D}}^{18} +23$ (c, 2 in CHCl_3)

>>Derivative: Me ester

CAS Registry Number: 66997-64-6

Molecular Formula: $\text{C}_9\text{H}_{18}\text{O}_3$

Molecular Weight: 174.239

Accurate Mass: 174.125595

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

Physical Description: Oil

Optical Rotation: $[\alpha]_{\text{D}}^{18} -27.1$ (c, 1 in CHCl_3)