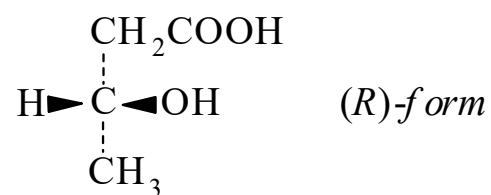




>>Entry Name: 3-Hydroxybutanoic acid, 9CI
ENTRY UNDER REVIEW



CAS Registry Number: 300-85-6

Related CAS Registry Numbers(s): 5864-66-4 25654-45-9 29435-48-1 35054-79-6 127604-16-4

Molecular Formula: C₄H₈O₃

Molecular Weight: 104.105

Accurate Mass: 104.047345

Percentage Composition: C 46.15%; H 7.75%; O 46.11%

Biological Source: Isol. from bacteria, in polymeric form

Use/Importance: The non-toxic homopolymer (*PHB*) and copolymer with 3-hydroxypentanoic acid (*Biopol*) are prod. microbially and used in biodegradable plastics applications. Reputed to have aphrodisiac properties

Aldrich: 16689-8

Sigma: H6376

>>Variant: (R)-form

CAS Registry Number: 625-72-9

Molecular Formula: C₄H₈O₃

Molecular Weight: 104.105

Accurate Mass: 104.047345

Percentage Composition: C 46.15%; H 7.75%; O 46.11%

Biological Source: Isol. from the spider *Linyphia triangularis*

Use/Importance: Sex pheromone

Physical Description: V. hygroscopic cryst.

Melting Point: Mp 49-50° (44-46°)

Optical Rotation: [α]_D -24.7 (c, 5 in H₂O). [α]_D¹⁶ -24.9

Solubility: V. sol. H₂O, EtOH; insol. C₆H₆

Fluka: 54920

>>Derivative: Na salt

CAS Registry Number: 13613-65-5

Melting Point: Mp 149-155°

Optical Rotation: [α]_D¹⁹ -11 (c, 10 in H₂O)

Aldrich: 29836-0

Fluka: 54963

Sigma: H0265

>>Derivative: Me ester

CAS Registry Number: 3976-69-0

Molecular Formula: C₅H₁₀O₃

Molecular Weight: 118.132

Accurate Mass: 118.062995

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

Boiling Point: Bp₁₃ 67-68.5°

Optical Rotation: [α]_D²⁵ -45.8 (c, 1.17 in CHCl₃)

Density: d₂₀²⁰ 1.06

Aldrich: 24315-9

Fluka: 54957

Sigma: M1016