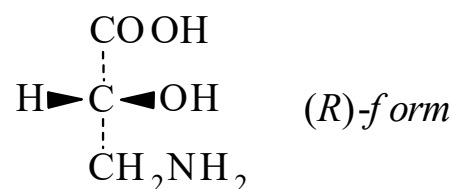




>>Entry Name: 3-Amino-2-hydroxypropanoic acid, 9CI

Synonym(s): Isoserine. 2-Hydroxy-β-alanine. 3-Aminolactic acid



CAS Registry Number: 565-71-9

Related CAS Registry Numbers(s): 105261-99-2 119326-39-5 133153-66-9 133153-75-0 133153-78-3 133268-45-8 133268-49-2

Molecular Formula: C₃H₇NO₃

Molecular Weight: 105.093

Accurate Mass: 105.042594

Percentage Composition: C 34.29%; H 6.71%; N 13.33%; O 45.67%

>>Variant: (R)-form

CAS Registry Number: 632-11-1

Molecular Formula: C₃H₇NO₃

Molecular Weight: 105.093

Accurate Mass: 105.042594

Percentage Composition: C 34.29%; H 6.71%; N 13.33%; O 45.67%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 199-201 dec.°

Optical Rotation: [α]_D²⁰+32.44 (H₂O)

>>Derivative: N-Benzoyl

Molecular Formula: C₁₀H₁₁NO₄

Molecular Weight: 209.201

Accurate Mass: 209.068809

Percentage Composition: C 57.41%; H 5.30%; N 6.70%; O 30.59%

Physical Description: Cryst. (EtOAc)

Melting Point: Mp 107-109°

Optical Rotation: [α]_D²⁰+10.52 (c, 10.26 in H₂O)

>>Variant: (S)-form

CAS Registry Number: 632-13-3

Extra CAS Registry Numbers(s): 81074-13-7

Molecular Formula: C₃H₇NO₃

Molecular Weight: 105.093

Accurate Mass: 105.042594

Percentage Composition: C 34.29%; H 6.71%; N 13.33%; O 45.67%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 199-201 dec.° (188-189°)

Optical Rotation: [α]_D²⁰-32.58 (c, 1 in H₂O)

>>Derivative: Me ester, hydrochloride

CAS Registry Number: 72185-81-0

Molecular Formula: C₄H₉NO₃

Molecular Weight: 119.12

Accurate Mass: 119.058244

Percentage Composition: C 40.33%; H 7.62%; N 11.76%; O 40.29%

Melting Point: Mp 104-105°

Optical Rotation: [α]_D²¹-19.2 (c, 1 in H₂O)

>>Derivative: Me ester, N-trityl

CAS Registry Number: 160233-40-9

Molecular Formula: C₂₃H₂₃NO₃

Molecular Weight: 361.44

Accurate Mass: 361.167794

Percentage Composition: C 76.43%; H 6.41%; N 3.88%; O 13.28%

Optical Rotation: [α]_D²⁴+17.2 (c, 1 in CHCl₃)