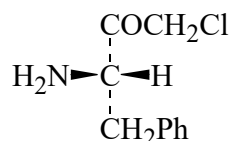




>>Entry Name: 3-Amino-1-chloro-4-phenyl-2-butanone, 9Cl



CAS Registry Number: 25487-45-0

Related CAS Registry Numbers(s): 36979-51-8 52735-73-6 149057-15-8

Molecular Formula: C₁₀H₁₂ClNO

Molecular Weight: 197.664

Accurate Mass: 197.060741

Percentage Composition: C 60.76%; H 6.12%; Cl 17.94%; N 7.09%; O 8.09%

>>Variant: (S)-form

CAS Registry Number: 52735-71-4

Molecular Formula: C₁₀H₁₂ClNO

Molecular Weight: 197.664

Accurate Mass: 197.060741

Percentage Composition: C 60.76%; H 6.12%; Cl 17.94%; N 7.09%; O 8.09%

>>Derivative: Hydrochloride

CAS Registry Number: 34351-19-4

Melting Point: Mp 169-170°

>>Derivative: Hydrobromide

CAS Registry Number: 25487-25-6

Physical Description: Cryst. (EtOH/Et₂O)

Melting Point: Mp 176° (174-175°)

Optical Rotation: $[\alpha]_D^{20} +30.2$ (c, 2 in 0.1M HCl)

>>Derivative: N-Benzyloxycarbonyl

CAS Registry Number: 26049-94-5

Molecular Formula: C₁₈H₁₈ClNO₃

Molecular Weight: 331.798

Accurate Mass: 331.097521

Percentage Composition: C 65.16%; H 5.47%; Cl 10.69%; N 4.22%; O 14.47%

Use/Importance: Inhibitor of carboxypeptidase Y

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 107-108° (105-106°)

Optical Rotation: $[\alpha]_D^{23} +30$ (c, 1 in CHCl₃)

>>Derivative: N-Me

CAS Registry Number: 52386-49-9

Molecular Formula: C₁₁H₁₄ClNO

Molecular Weight: 211.69

Accurate Mass: 211.076391

Percentage Composition: C 62.41%; H 6.67%; Cl 16.75%; N 6.62%; O 7.56%

Melting Point: Mp 145° (dec.) (as hydrochloride). Mp 167° (dec.) (as hydrobromide)

Optical Rotation: $[\alpha]_D^{20} +76.1$ (c, 2 in 0.1M HCl) (as hydrobromide)

Other Data: CAS no. refers to hydrochloride

>>Derivative: N-Me, N-benzyloxycarbonyl

CAS Registry Number: 52386-45-5

Molecular Formula: C₁₉H₂₀ClNO₃

Molecular Weight: 345.825

Accurate Mass: 345.113171

Percentage Composition: C 65.99%; H 5.83%; Cl 10.25%; N 4.05%; O 13.88%

Physical Description: Syrup

References: