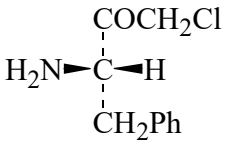
>>**Entry Name: 3-Amino-1-chloro-4-phenyl-2-butanone,** 9Cl



CAS Registry Number: 25487-45-0
Related CAS Registry Numbers(s): 36979-51-8 52735-73-6 149057-15-8

Molecular Formula: $C_{10}H_{12}ClNO$
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: $C_{10}H_{12}ClNO$
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. ($EtOH/Et_2O$)
Melting Point: Mp 176° (174-175°)
Optical Rotation: $[\alpha]_D^{20}$+30.2 (c, 2 in 0.1*M* HCl)

>>**Derivative:** *N*-Benzyloxycarbonyl

CAS Registry Number: 26049-94-5
Molecular Formula: $C_{18}H_{18}ClNO_3$
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 $CHCl_3$)

>>**Derivative:** *N*-Me

CAS Registry Number: 52386-49-9
Molecular Formula: $C_{11}H_{14}ClNO$
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 0.1*M* HCl) (as hydrobromide)
Other Data: CAS no. refers to hydrochloride

>>**Derivative:** *N*-Me, *N*-benzyloxycarbonyl

CAS Registry Number: 52386-45-5
Molecular Formula: $C_{19}H_{20}ClNO_3$
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: