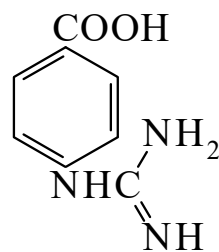




>>Entry Name: 4-[(Aminoiminomethyl)amino]benzoic acid, 9Cl

Synonym(s): *p*-Guanidinobenzoic acid, 8Cl



CAS Registry Number: 16060-65-4

Related CAS Registry Numbers(s): 76472-28-1

Molecular Formula: C₈H₉N₃O₂

Molecular Weight: 179.178

Accurate Mass: 179.069477

Percentage Composition: C 53.63%; H 5.06%; N 23.45%; O 17.86%

Melting Point: Mp 260-270 dec.°

>>Derivative: Hydrochloride

CAS Registry Number: 42823-46-1

Physical Description: Cryst. (H₂O)

Melting Point: Mp 268 dec.°

Aldrich: 37496-2

Fluka: 51005

Sigma: G4131

>>Derivative: Ph ester

CAS Registry Number: 35695-21-7

Molecular Formula: C₁₄H₁₃N₃O₂

Molecular Weight: 255.276

Accurate Mass: 255.100777

Percentage Composition: C 65.87%; H 5.13%; N 16.46%; O 12.54%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 340° (dec.)

>>Derivative: 4-Nitrophenyl ester

CAS Registry Number: 21658-26-4

Extra CAS Registry Numbers(s): 19135-17-2

Molecular Formula: C₁₄H₁₂N₄O₄

Molecular Weight: 300.273

Accurate Mass: 300.085856

Percentage Composition: C 56.00%; H 4.03%; N 18.66%; O 21.31%

Use/Importance: Trypsin inhibitor

Melting Point: Mp 227° (as hydrochloride)

>>Derivative: 4-(Aminosulfonyl)phenyl ester

Synonym(s): ONO 3307

CAS Registry Number: 76472-29-2

Molecular Formula: C₁₄H₁₄N₄O₄S

Molecular Weight: 334.355

Accurate Mass: 334.073576

Percentage Composition: C 50.29%; H 4.22%; N 16.76%; O 19.14%; S 9.59%

Use/Importance: Protease inhibitor. Shows protective effect in animal models of acute pancreatitis

Melting Point: Mp 225° (as methanesulfonate)

Other Data: CAS No. refers to methanesulfonate

References: