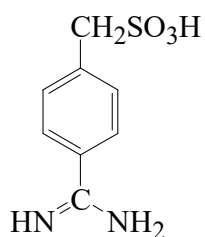




>>Entry Name: 4-(Aminoiminomethyl)benzenemethanesulfonic acid, 9Cl

Synonym(s): (4-Amidinophenyl)methanesulfonic acid



Molecular Formula: C₈H₁₀N₂O₃S

Molecular Weight: 214.245

Accurate Mass: 214.041213

Percentage Composition: C 44.85%; H 4.70%; N 13.08%; O 22.40%; S 14.97%

>>Derivative: Me ester

CAS Registry Number: 60560-97-6

Extra CAS Registry Numbers(s): 60560-98-7

Molecular Formula: C₉H₁₂N₂O₃S

Molecular Weight: 228.271

Accurate Mass: 228.056863

Percentage Composition: C 47.36%; H 5.30%; N 12.27%; O 21.03%; S 14.05%

Melting Point: Mp 312° (as trifluoroacetate salt)

>>Derivative: Fluoride

CAS Registry Number: 71933-13-6

Extra CAS Registry Numbers(s): 74938-88-8

Molecular Formula: C₈H₉FN₂O₂S

Molecular Weight: 216.236

Accurate Mass: 216.036876

Percentage Composition: C 44.44%; H 4.20%; F 8.79%; N 12.96%; O 14.80%; S 14.83%

Use/Importance: Irreversible inhibitor of serine proteases

Melting Point: Mp 190-191° (as hydrochloride)

References:

Wong, S.C. *et al.*, *Arch. Biochem. Biophys.*, 1976, **176**, 113-118, (*Me ester, synth*)

Laura, R. *et al.*, *Biochemistry*, 1980, **19**, 4859-4864, (*fluoride, synth, ir, pmr, use*)