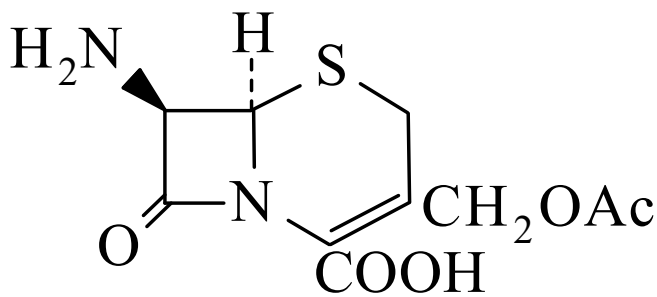




>>Entry Name: 7-Aminocephalosporanic acid

Synonym(s): 7-ACA



CAS Registry Number: 957-68-6

Molecular Formula: C₁₀H₁₂N₂O₅S

Molecular Weight: 272.281

Accurate Mass: 272.046693

Percentage Composition: C 44.11%; H 4.44%; N 10.29%; O 29.38%; S 11.78%

Biological Source: Prod. by chemical cleavage or enzymic hydrol. of Cephalosporin C

Use/Importance: Starting material for synth. of many semisynthetic cephalosporins

Physical Description: Cryst.

Aldrich: 19114-0

Fluka: 7300

Sigma: A3392

>>Derivative: *tert*-Butyl ester

CAS Registry Number: 6187-87-7

Extra CAS Registry Numbers(s): 33610-06-9

Molecular Formula: C₁₄H₂₀N₂O₅S

Molecular Weight: 328.388

Accurate Mass: 328.109293

Percentage Composition: C 51.21%; H 6.14%; N 8.53%; O 24.36%; S 9.76%

Use/Importance: Synthon for cephalosporins contg. an acid-labile *tert*-butyl ester grouping

Physical Description: Cryst. (EtOAc)

Melting Point: Mp 114-115°

>>Derivative: Diphenylmethyl ester

CAS Registry Number: 27266-61-1

Molecular Formula: C₂₃H₂₂N₂O₅S

Molecular Weight: 438.503

Accurate Mass: 438.124943

Percentage Composition: C 63.00%; H 5.06%; N 6.39%; O 18.24%; S 7.31%

Physical Description: Cryst. (THF/Et₂O)

Melting Point: Mp 125-127° (45-46°)

Other Data: The lower Mp appears to be erroneous

>>Derivative: *O*-De-Ac

Synonym(s): 7-Amino-3-(hydroxymethyl)-3-cephem-4-carboxylic acid. 7-Aminodeacetylcephalosporanic acid

CAS Registry Number: 15690-38-7

Extra CAS Registry Numbers(s): 14441-14-6

Molecular Formula: C₈H₁₀N₂O₄S

Molecular Weight: 230.244

Accurate Mass: 230.036128

Percentage Composition: C 41.73%; H 4.38%; N 12.17%; O 27.80%; S 13.93%

Biological Source: Prod. by *Acremonium chrysogenum*

Physical Description: Powder + H₂O (as Na salt)

References: