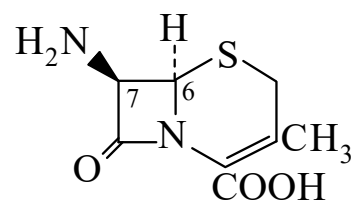




>>Entry Name: 7-Amino-3-methyl-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 9Cl

Synonym(s): 7-Amino-3-methyl-3-cephem-4-carboxylic acid. 7-Aminodeacetoxycephalosporanic acid. 7-ADCA



CAS Registry Number: 26395-99-3

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%

>>Variant: (6*R*,7*R*)-form

CAS Registry Number: 22252-43-3

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%

Biological Source: Prod. by *Acremonium chrysogenum*

Use/Importance: Starting material for cephem antibiotics

Melting Point: Mp 241-242°

Optical Rotation: $[\alpha]_D^{18} +111$ (c, 0.175 in DMSO)

Sigma: A8398

>>Derivative: *N*-Ac, Me ester

CAS Registry Number: 40818-81-3

Source/Synthesis: Semisynthetic

Physical Description: Needles (CH₂Cl₂/petrol)

Melting Point: Mp 214-216°

Optical Rotation: $[\alpha]_D^{18} +181$ (c, 0.138 in CHCl₃)

>>Derivative: *N*-(Phenylacetyl)

CAS Registry Number: 27255-72-7

Molecular Formula: C₁₆H₁₆N₂O₄S

Molecular Weight: 332.379

Accurate Mass: 332.083078

Percentage Composition: C 57.82%; H 4.85%; N 8.43%; O 19.25%; S 9.65%

Physical Description: Cryst. (2-propanol/petrol)

Melting Point: Mp 198-200°

>>Derivative: *N*-(Phenoxyacetyl)

CAS Registry Number: 10209-11-7

Molecular Formula: C₁₆H₁₆N₂O₅S

Molecular Weight: 348.379

Accurate Mass: 348.077993

Percentage Composition: C 55.16%; H 4.63%; N 8.04%; O 22.96%; S 9.20%

Physical Description: Cryst. (EtOAc/petrol)

Melting Point: Mp 186-188°

>>Derivative: 10-Acetoxy

see 7-Aminocephalosporanic acid, [CKN38-P](#)

References: