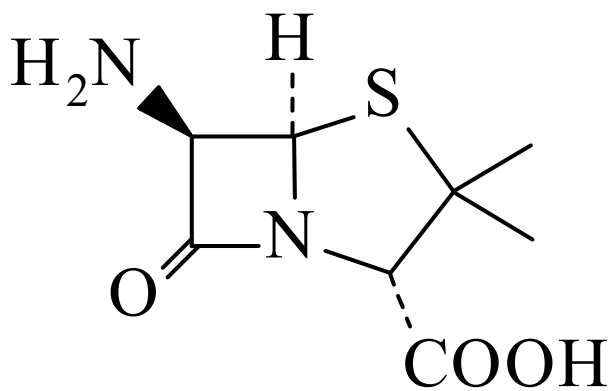




>>Entry Name: 6-Aminopenicillanic acid

Synonym(s): Penicin. 6-APA



CAS Registry Number: 551-16-6

Molecular Formula: C₈H₁₂N₂O₃S

Molecular Weight: 216.26

Accurate Mass: 216.056863

Percentage Composition: C 44.43%; H 5.59%; N 12.95%; O 22.19%; S 14.83%

Biological Source: Prod. by enzymic hydrol. of benzyl- or phenoxymethylpenicillins. Also prod. as metab. prod. of several penicillin-producing fungi, esp. when side-chain precursors are absent.

Use/Importance: Precursor of semisynthetic penicillins

Melting Point: Mp 208-209 dec.°

Optical Rotation: [α]_D³¹+273 (c, 1.2 in 0.1M HCl)

pKa Value: pK_{a1} 2.3; pK_{a2} 4.92 (25°, H₂O)

Hazard & Toxicity: LD₅₀ (mus, ipr) >1000 mg/kg

Aldrich: A7090-9

Fluka: 9070

Sigma: A1005

>>Derivative: Me ester

Molecular Formula: C₉H₁₄N₂O₃S

Molecular Weight: 230.287

Accurate Mass: 230.072513

Percentage Composition: C 46.94%; H 6.13%; N 12.16%; O 20.84%; S 13.92%

Physical Description: Cryst. (Me₂CO)

Melting Point: Mp 177.5-178°

Optical Rotation: [α]_D²⁸+288 (c, 1.1 in butyl acetate)

>>Derivative: 4-Oxide

CAS Registry Number: 4888-97-5

Molecular Formula: C₈H₁₂N₂O₄S

Molecular Weight: 232.26

Accurate Mass: 232.051778

Percentage Composition: C 41.37%; H 5.21%; N 12.06%; O 27.55%; S 13.81%

Physical Description: Powder

Melting Point: Mp 190-193 dec.°

>>Derivative: 6-Deamino-6 β -bromo

References: