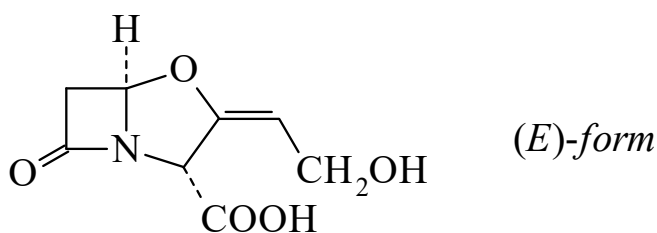




>>Entry Name: Clavulanic acid, BAN, INN

Synonym(s): 3-(2-Hydroxyethylidene)-7-oxo-4-oxa-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 9CI. Clavubactam



Related CAS Registry Numbers(s): 60802-63-3 61177-42-2 61177-43-3 61177-44-4 61177-46-6 61970-10-3 66428-09-9 67529-22-0 79198-29-1

Molecular Formula: C₈H₉NO₅

Molecular Weight: 199.163

Accurate Mass: 199.048074

Percentage Composition: C 48.25%; H 4.55%; N 7.03%; O 40.17%

General Statement: β -Lactam antibiotic

Calculated Log P Data: Log P -1.51 (calc)

>>Variant: (E)-form

Synonym(s): Isoclavulanic acid

CAS Registry Number: 62319-53-3

Molecular Formula: C₈H₉NO₅

Molecular Weight: 199.163

Accurate Mass: 199.048074

Percentage Composition: C 48.25%; H 4.55%; N 7.03%; O 40.17%

>>Derivative: Me ester

CAS Registry Number: 66428-10-2

Molecular Formula: C₉H₁₁NO₅

Molecular Weight: 213.19

Accurate Mass: 213.063724

Percentage Composition: C 50.71%; H 5.20%; N 6.57%; O 37.52%

Physical Description: Oil

Optical Rotation: $[\alpha]_D^{22} +38.4$ (c, 1.77 in MeOH)

>>Derivative: *p*-Bromobenzyl ester

CAS Registry Number: 60802-62-2

Molecular Formula: C₁₅H₁₄BrNO₅

Molecular Weight: 368.183

Percentage Composition: C 48.93%; H 3.83%; Br 21.70%; N 3.80%; O 21.73%

Physical Description: Thin rods (CH₂Cl₂/CCl₄)

Melting Point: Mp 134-134.5°

Optical Rotation: $[\alpha]_D^{25} +23$ (c, 1.16 in MeOH)

>>Variant: (Z)-form

Synonym(s): MM 14151. BRL 14440. Antibiotic MM 14151. Antibiotic 3008B

CAS Registry Number: 58001-44-8

Molecular Formula: C₈H₉NO₅

Molecular Weight: 199.163

Accurate Mass: 199.048074

Percentage Composition: C 48.25%; H 4.55%; N 7.03%; O 40.17%

Biological Source: Metab. of *Streptomyces clavuligerus*, *Streptomyces jumonjinensis* and *Streptomyces katsurahamanus*

Biological Use/Importance: Potent inhibitor of β -lactamases produced by gram-positive and -negative bacteria. Weak antibacterial activity. Enhances antibiotic activity of penicillins and cephalosporins when co-administered

Physical Description: Unstable oil

>>Derivative: Na salt

CAS Registry Number: 57943-81-4

Physical Description: Feathery needles + 4H₂O (Me₂CO aq.)

Melting Point: Mp 68°