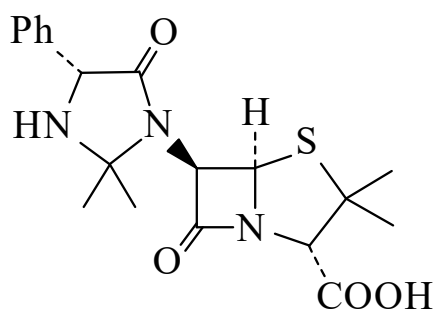




>>>**Entry Name:** Hetacillin, BAN, INN, USAN

Synonym(s): 6-(2,2-Dimethyl-5-oxo-4-phenyl-1-imidazolidinyl)penicillanic acid. Etacillin. Phenazacillin. Versapen. Versatrex. BRL 804. Antibiotic BRL 804. BL P804. Many other names



CAS Registry Number: 3511-16-8

Related CAS Registry Numbers(s): 60252-40-6

Molecular Formula: C₁₉H₂₃N₃O₄S

Molecular Weight: 389.474

Accurate Mass: 389.140927

Percentage Composition: C 58.59%; H 5.95%; N 10.79%; O 16.43%; S 8.23%

Source/Synthesis: Semisynthetic penicillin (acetone adduct of Ampicillin)

Biological Use/Importance: Orally absorbed antibiotic

Physical Description: Cryst. (5-methyl-2-hexanone aq.)

Melting Point: Mp 182.8-183.9 dec.°

Optical Rotation: [α]_D²⁵+366 (c, 1.0 in Py)

Solubility: Sol. DMF, DMSO

Calculated Log P Data: Log P 1.51 (uncertain value) (calc)

Sigma: H0384

>>>**Derivative:** K salt

Synonym(s): Hetacillin potassium, JAN, USAN. Natacillin. Uropen

CAS Registry Number: 5321-32-4

Sigma: H0509

>>>**Derivative:** Me ester

Physical Description: Cryst. (CCl₄)

Melting Point: Mp 101.5-102°

>>>**Derivative:** Methoxymethyl ester

Synonym(s): Sarpicillin, INN, USAN. BL-P 1761. Antibiotic BL-P 1761

CAS Registry Number: 40966-79-8

Molecular Formula: C₂₁H₂₇N₃O₅S

Molecular Weight: 433.527

Accurate Mass: 433.167142

Percentage Composition: C 58.18%; H 6.28%; N 9.69%; O 18.45%; S 7.40%

Biological Use/Importance: Semisynthetic antibiotic used against *Haemophilus influenzae*. Prodrug for Ampicillin giving CNS penetration

Development Status: Never marketed

Calculated Log P Data: Log P 3.77 (uncertain value) (calc)

References:

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Negwer, M., *Organic-Chemical Drugs and their Synonyms*, 6th edn., Akademie-Verlag, 1987, 5339, (*synonyms*)
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