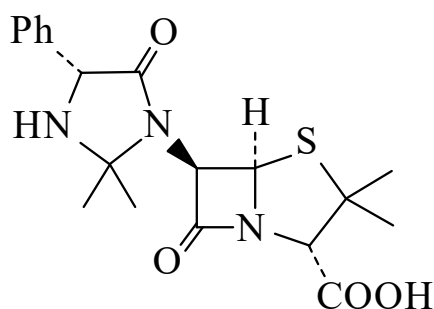




>>>**Entry Name:** Hetacillin, BAN, INN, USAN

**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:** C<sub>19</sub>H<sub>23</sub>N<sub>3</sub>O<sub>4</sub>S

**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:** [ $\alpha$ ]<sub>D</sub><sup>25</sup>+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. (CCl<sub>4</sub>)

**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:** C<sub>21</sub>H<sub>27</sub>N<sub>3</sub>O<sub>5</sub>S

**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:

- Hardcastle, G. *et al.*, *J.O.C.*, 1966, **31**, 897, (*synth, cryst struct*)  
Kirby, W.M.M. *et al.*, *Ann. N.Y. Acad. Sci.*, 1967, **145**, 291, (*pharmacol*)  
Ueda, Y. *et al.*, *J. Antibiot., Ser. B*, 1967, **20**, 206, (*pharmacol*)  
Johnson, D. *et al.*, *Tet. Lett.*, 1968, 1903  
*U.S. Pat.*, 1976, 3 996 236; *CA*, **86**, 155640, (*Sarpicillin*)  
Ferres, H., *Chem. Ind. (London)*, 1980, 435  
Negwer, M., *Organic-Chemical Drugs and their Synonyms*, 6th edn., Akademie-Verlag, 1987, 5339, (*synonyms*)  
*Martindale, The Extra Pharmacopoeia*, 30th edn., Pharmaceutical Press, 1993, 172