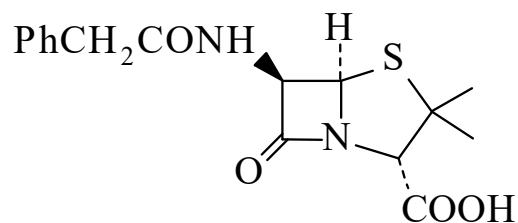




>>Entry Name: Benzylpenicillin, BAN, INN

Synonym(s): 6-(Phenylacetamido)penicillanic acid. Penicillin G. Penicillin II. Phenylacetylpenin. Benzylpenicillinic acid. Cristapen. Ursopen. Cilopen. Novocillin. BRL 3000



CAS Registry Number: 61-33-6

Related CAS Registry Numbers(s): 1406-07-1 5928-83-6 6130-64-9 41372-02-5

Molecular Formula: C<sub>16</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S

Molecular Weight: 334.395

Accurate Mass: 334.098728

Percentage Composition: C 57.47%; H 5.43%; N 8.38%; O 19.14%; S 9.59%

Biological Source: Antibiotic from *Penicillium* spp. and also other fungal spp.

Biological Use/Importance: Shows activity against gram-positive bacteria. Starting material for production of 6-Aminopenicillanic acid. Used as a 5% soln. in acetate buffer for gravimetric detn. of Fe

Physical Description: Cryst.

Optical Rotation:  $[\alpha]_D +282$  (EtOH)

Calculated Log P Data: Log P 1.68 (uncertain value) (calc)

Other Data: Production enhanced by adding Phenylacetic acid to fermentation

Hazard & Toxicity: Hypersensitivity reactions and other adverse effects reported when used therapeutically. LD<sub>50</sub> (rat, orl) 8000 mg/kg

Sigma: B2751

>>Derivative: Na salt

Synonym(s): Penicillin G sodium, USAN

CAS Registry Number: 69-57-8

Physical Description: Needles (butanol aq.)

Melting Point: Mp 215 dec.°

Optical Rotation:  $[\alpha]_D^{25} +301$  (H<sub>2</sub>O)

Solubility: Sol. H<sub>2</sub>O, MeOH

Hazard & Toxicity: LD<sub>50</sub> (rat, orl) 6916 mg/kg. Exp. reprod. and teratogenic effects

Fluka: 13752

Sigma: P3414

>>Derivative: K salt

Synonym(s): Penicillin G potassium, USAN. Cilloral. Liquapen. Sugracillin. Pentids. Many other names

CAS Registry Number: 113-98-4

Physical Description: Needles (butanol aq.)

Melting Point: Mp 214-217 dec.°

Optical Rotation:  $[\alpha]_D^{22} +285$  (H<sub>2</sub>O)

Solubility: Sol. H<sub>2</sub>O

Hazard & Toxicity: LD<sub>50</sub> (rat, orl) 6700 mg/kg

Fluka: 13750

Sigma: P5375

>>Derivative: Procaine salt (1:1)

Synonym(s): Penicillin G procaine, USAN. Procaine penicillin, BAN. Abbocillin. Aquacillin. Duracillin. Eskacillin. Duphpen. Hydracillini. Vitablend. Hostacillin. Many other names

CAS Registry Number: 54-35-3

Biological Use/Importance: Antibiotic for injection

Melting Point: Mp 129-130°

Optical Rotation:  $[\alpha]_D^{25} +173$  (50% Me<sub>2</sub>CO aq.)