



Formula: C₁₆H₁₉N₃O₄S

MW: 349.41

Salt: 3H₂O

CAS: 69-53-4, 7177-48-2

TNP NUMBER: TNP00228

MDL NUMBER: MFCD00249428

IUPAC: (2S,5R,6R)-6-(2-amino-2-phenylacetyl-amino)-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid

Smiles:

c1ccc(cc1)C(C(N[C@@H]1(C(N2[C@@H]1S[C@@]([C@@H]2(C(O)=O))(C)C)=O)=O)N

THERAPEUTIC CATEGORY: Antibacterial

VET THERAP CATEGORY: Antibacterial

REFERENCE: Merck 13,591

SOURCE: Semi-synthetic orally active antibiotic structurally related to penicillin. Amino derivative of penicillin

ACCEPTORS: 4

DONORS: 4

ROTATION BONDS: 3

N+O: 7

Chiral Centers: 4

LogP: 0.34

LogS: -3.3

LIPINSKI: 4

Synonyms:

amcap;amcill;aminobenzylpenicillintrihydrate;amperil;ampichel;ampinova;amplin;cymbi

CAS:7177-48-2

MF:C16H25N3O7S

MW:403.45

EINECS:200-709-7

Product Categories:Antibiotics for Research and Experimental Use;beta-Lactams (Antibiotics for Research and Experimental Use);Biochemistry Ampicillin

Chemical Properties: mp 208 C (dec.)(lit.) refractive index 265 (C=0.1, H2O) storage temp. 2-8C solubility NH4OH 1 M: 50 mg/mL, clear, colorless Water Solubility 0.1-1 g/100 mL at 21 C Merck 586

CAS DataBase Reference: 7177-48-2(

CAS DataBase Reference:) EPA Substance Registry System4-Thia-1-azabicyclo(3.2.0)heptane-2-carboxylic acid, 6-[[[(2R)-aminophenylacetyl] amino]-3,3-dimethyl-7-oxo-, trihydrate, (2S,5R,6R)-(7177-48-2) Xn,Xi Risk Statements 36/37/38-42/43 Safety Statements 22-26-36/37-36 WGK Germany 2 RTECS XH8425000 F 3-10 Ampicillin Ampicillin

Usage And Synthesis:

Chemical Properties: Crystalline General DescriptionOdorless white microcrystalline powder with a bitter taste. A 0.25% solution in water has a pH of 3.5 to 5.5. Air & Water ReactionsSlightly soluble in water. Reactivity ProfileAmpicillin absorbs insignificant amounts of moisture at 77 F and relative humidities up to approximately 80%, but under damper conditions Ampicillin absorbs significant amounts. A pH-rate profile reveals specific-acid- and specific-base- catalyzed hydrolysis. The pH of maximum stability is 5.8. Fire HazardFlash point data for Ampicillin are not available; however, Ampicillin is probably combustible. Ampicillin



