



Formula: C₈H₁₂N₂O₃S

MW: 216.26

CAS: 551-16-6

MDL: MFCD03225429

TNP: TNP00465

(2S,5R,6R)-6-AMINO-3,3-DIMETHYL-7-OXO-4-THIA-1-AZABICYCLO[3.2.0]HEPTANE-2-CARBOXYLIC ACID;
(2S,5R,6R)-6-AMINO-3,3-DIMETHYL-7-OXO-4-THIA-1-AZABICYCLO-[3.2.0]HEPTANE-2-CARBOXYLIC ACID;
6-AMINO-2,2-DIMETHYL-5-OXOPERHYDROAZETO[2,1-B][1,3]THIAZOLE-3-CARBOXYLIC A



LogP: -7.34

LogS: -1

Acceptors: 3

Donors: 3

Rotation Bonds: 1

Chiral Centers: 3

N+O: 5

LIPINSKY: 4

Info: 6-Aminopenicillanic acid 96%, Obtained from cultures of *Penicillium Chrysogenum*

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

Smiles: N12C(SC([C@@H]2C(=O)O)(C)C)C(C1=O)N

Specification: Organic acids; Antibiotics for Research and Experimental Use; beta-Lactams (Antibiotics for Research and Experimental Use); Biochemistry 6-Aminopenicillanic acid
Chemical Properties:

mp 198-200 C (dec.)(lit.) alpha 276.3