



Formula: C<sub>31</sub>H<sub>41</sub>N<sub>7</sub>O<sub>6</sub>

MW: 607.71

CAS: 9076-44-2

MDL: MFCD06668138

TNP: TNP00281

(S)-1-CARBOXY-2-PHENYLETHYL]-CARBAMOYL-ALPHA-[2-AMIDOHXAHYDRO-4(S)-PYRIMIDYL]- (S)-GLYCYL-[A = LEU; B = VAL; OR C = ILE]-PHENYLALANINAL;  
(S)-1-CARBOXY-2-PHENYLETHYL)-CARBAMOYL-ALPHA-[2-IMINOHEXAHYDRO-4(S)-PYRIMIDYL]- (S)-GLYCYL-X-PHENYLALANINAL; [(S)-1-CARBO



LogP: 8.06

LogS: -7.71

Acceptors: 6

Donors: 8

Rotation Bonds: 14

Chiral Centers: 5

N+O: 13

LIPINSKY: 1

Info: Microbial, A mixture of A (major), B and C components. A: X=Leu; B: X=Val; C: X=Ile

IUPAC: 2-[(N-[(2-imino(1,3-diazaperhydroin-4-yl))[N-(3-methyl-1-[N-[2-oxo-1-benzylethyl]carbamoyl]butyl)carbamoyl]methyl]carbamoyl)amino]-3-phenylpropanoic acid

Smiles:

c1(ccccc1)CC(NC(NC(C(NC(C(NC(Cc1ccccc1)C=O)=O)CC(C)C)=O)C1CCNC(N1)=N)=O)C(O)=O

Specification: CHYMOSTATIN Chemical Properties:

storage temp. -20C solubility DMSO: 10 mM Stock solutions stable for months at -20 C. Safety Information Hazard Codes Xi Risk Statements 36/37/38 Safety Statements 22-24/25-36-26 WGK Germany 3 RTECS GC3047700 F 10-21 CHYMOSTATIN Usage And Synthesis CHYMOSTATIN