

(4R)-4-[(2S)-2-{[(5R)-2-[(1S,2R)-1-AMINO-2-METHYLBUTYL]-4,5-DIHYDRO-1,3-THIAZOL-5-YL]FORMAMIDO}-4-METHYLPENTANAMIDO]-4-{[(1S,2R)-1-{[(3S,6R,9S,12R,15S,18R,21S)-18-(3-AMINOPROPYL)-12-BENZYL-15-[(2R)-BUTAN-2-YL]-3-(CARBAMOYLMETHYL)-6-(CARBOXYMETHYL)-9-[(1H-IMIDAZOL-5-YL)METHYL]-2,5,8,11,14,17,20-HEPTAOXO-1,4,7,10,13,16,19-HEPTAAZACYCLOPENTACOSAN-21-YL]CARBAMOYL}-2-METHYLBUTYL]CARBAMOYL}BUTANOIC ACID

Catalog Id:

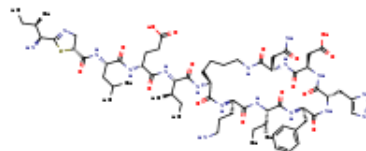
MM1405874

IUPAC:

BACITRACIN

CAS Number:

1405-87-4



More Information:

Molecular Weight: 1422.71

Formula: C₆₆H₁₀₃N₁₇O₁₆S

SMILES:

CC[C@H](C)[C@H](N)C1=NC[C@@H](S1)C(=O)N[C@@H](CC(C)C)C(=O)N[C@H](CCC(O)=O)C(=O)N[C@@H]([C@H](C)CC)C(=O)N[C@H]1CC

Preferred IUPAC Name: (4R)-4-[(2S)-2-{[(5R)-2-[(1S,2R)-1-AMINO-2-METHYLBUTYL]-4,5-DIHYDRO-1,3-THIAZOL-5-YL]FORMAMIDO}-4-METHYLPENTANAMIDO]-4-{[(1S,2R)-1-{[(3S,6R,9S,12R,15S,18R,21S)-18-(3-AMINOPROPYL)-12-BENZYL-15-[(2R)-BUTAN-2-YL]-3-(CARBAMOYLMETHYL)-6-(CARBOXYMETHYL)-9-[(1H-IMIDAZOL-5-YL)METHYL]-2,5,8,11,14,17,20-HEPTAOXO-1,4,7,10,13,16,19-HEPTAAZACYCLOPENTACOSAN-21-YL]CARBAMOYL}-2-METHYLBUTYL]CARBAMOYL}BUTANOIC ACID

InChIKey: InChIKey=MNJKVJAYSVAQLU-GTLFSKLRSA-N