

{[5-(6-AMINO-9H-PURIN-9-YL)-4-HYDROXY-2-({[HYDROXY({HYDROXY[3-HYDROXY-2,2-DIMETHYL-3-({2-[(2-SULFANYLETHYL)CARBAMOYL]ETHYL}CARBAMOYL)PROPOXY]PHOSPHORYL}OXY)PHOSPHORYL]OXY}METHYL)OXOLAN-3-YL]OXY}PHOSPHONIC ACID

Catalog Id:

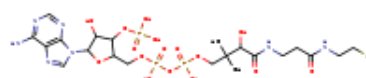
MM85610

IUPAC:

COENZYME A

CAS Number:

85-61-0



More Information:

Molecular Weight: 767.53

Formula: C₂₁H₃₆N₇O₁₆P₃S

SMILES: CC(C)(COP(O)(=O)OP(O)(=O)OCC1OC(C(O)C1OP(O)(O)=O)N1C=NC2=C1N=CN=C2N)C(O)C(=O)NCCC(=O)NCCS

Preferred IUPAC Name: {[5-(6-AMINO-9H-PURIN-9-YL)-4-HYDROXY-2-({[HYDROXY({HYDROXY[3-HYDROXY-2,2-DIMETHYL-3-({2-[(2-SULFANYLETHYL)CARBAMOYL]ETHYL}CARBAMOYL)PROPOXY]PHOSPHORYL}OXY)PHOSPHORYL]OXY}METHYL)OXOLAN-3-YL]OXY}PHOSPHONIC ACID

InChIKey: InChIKey=RGJOEKWQDUBAIZ-UHFFFAOYNA-N