

Typical Product Specifications & Properties

4-(2'-Carboxyphenyl)-4-Oxobutyryl-Coenzyme A Ester

CAS Number: : 97226-61-4

Specifications	Limits
SMILES	<chem>O=[P@@](O[P@@](OC[C@@H]1[C@@H](OP(O)(=O)O)[C@@H]([C@@H](n2cnc3c(ncnc23)N)O1)O)(=O)O)(OCC([C@@H](O)C(NCCC(NCCSC(CCC(c1c(cccc1)C(=O)O)=O)=O)=O)=O)=O)=O)=O=C(C)C)O</chem>
InChI	KVAQAPQXOXTRAE-UHFFFAOYSA-N
InChIKey	1S/C32H44N7O20P3S/c1-32(2,26(44)29(45)35-10-9-21(41)34-1112-63-22(42)8-7-19(40)17-5-3-4-6-18(17)31(46)47)14-56-62(53,54)59-61(51,52)55-13-20-25(58-60(48,49)50)24(43)30(57-20)39-16-38-23-27(33)36-15-37-28(23)39/h3-6,15-16,20,24-26,30,43-44H,7-14H2,1-