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Typical Product Specifications & Properties

3-Chloropropionyl-Coenzyme A

CAS Number: : 96212-36-1

Specifications	Limits
SMILES	<chem>OP(O[C@@H]1[C@@H](O[C@@H]([C@@H]1O)n1cnc2c(N)ncnc12)CO[P@@](=O)(O)O[P@@](=O)(O)OCC(C)(C)[C@@H](C(NCCC(NCCSC(=O)CCCI)=O)=O)O)(O)=O</chem>
InChI	LBJZPAYTKZKLLL-UHFFFAOYSA-N
InChIKey	1S/C24H39CIN7O17P3S/c1-24(2,19(36)22(37)28-6-4-14(33)27-7-8-53-15(34)3-5-25)10-46-52(43,44)49-51(41,42)45-9-13-18(48-50(38,39)40)17(35)23(47-13)32-12-31-16-20(26)29-11-30-21(16)32/h11-13,17-19,23,35-36H,3-10H2,1-2H3,(H,27,33)(H,28,37)(H,41,42)(H,43,4



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