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Typical Product Specifications & Properties

beta-Diphosphopyridinenucleotide

CAS Number: : 53-84-9

Specifications	Limits
Molecular weight	663.43
EINECS	200-184-4
SMILES	<chem>n1(c2c(c(ncn2)N)nc1)[C@@H]1O[C@H](CO[P@@](OP(OC[C@H]2O[C@@H]([n+]3cc(ccc3)C(N)=O)[C@@H]([C@@H]2O)O)(=O)[O-])(O)=O)[C@H]([C@H]1O)O</chem>
InChI	BAWFJGJZ GIEFAR-NNYOXOHSSA-N
InChIKey	1S/C21H27N7O14P2/c22-17-12-19(25-7-24-17)28(8-26-12)21-16(32)14(30)11(41-21)6-39-44(36,37)42-43(34,35)38-5-10-13(29)15(31)20(40-10)27-3-1-2-9(4-27)18(23)33/h1-4,7-8,10-11,13-16,20-21,29-32H,5-6H2,(H5-,22,23,24,25,33,34,35,36,37)/t10-,11-,13-,14-,15-,1
log P (octanol-water)	-3.680
Atmospheric OH Rate Constant	3.18E-10 cm ³ /molecule-sec



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415 Huguenot Street, New Rochelle, New York 10801

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