

Product Information

NADPH tetracyclohexanamine

Cat. No.: X25-06-LY849

Size: 5 mg; 10 mg; 25 mg; 50 mg; 100 mg

CAS Number: 100929-71-3

Compound CID: 71312102

Synonym: 100929-71-3;

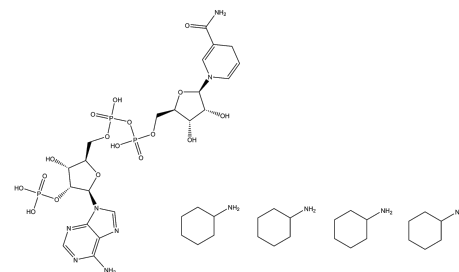
[[*(2R,3R,4R,5R*

)-5-(6-Aminopurin-9-yl)-3-hydroxy-4-phosphonooxyoxolan-2-yl]methoxy-hydroxyphosphoryl]

[[*(2R,3S,4R,5R)*-5-(3-Carbamoyl-4*H*-pyridin-1-yl)-3,4-dihydroxyoxolan-2-yl]methyl hydrogen phosphate;cyclohexanamine; NADPH Tetracyclohexanamine; NADPH (tetracyclohexanamine);

[[*(2R,3S,4R,5R)*-5-(3-Carbamoyl-4*H*-pyridin-1-yl)-3,4-dihydroxyoxolan-2-yl]methyl hydrogen phosphate

This product is for research use only and is not intended for diagnostic use.



Product Information

Description	NADPH tetracyclohexanamine is a NADPH derivative containing tetracyclohexylamine, which can be used in a specific chemical synthesis.
Molecular Weight	1142.12
Molecular Formula	C ₄₅ H ₈₂ N ₁₁ O ₁₇ P ₃
IUPAC Name	[[<i>(2R,3R,4R,5R)</i> -5-(6-Aminopurin-9-yl)-3-hydroxy-4-phosphonooxyoxolan-2-yl]methoxy-hydroxyphosphoryl] [[<i>(2R,3S,4R,5R)</i> -5-(3-carbamoyl-4 <i>H</i> -pyridin-1-yl)-3,4-dihydroxyoxolan-2-yl]methyl hydrogen phosphate;cyclohexanamine
InChI	InChI=1S/C21H30N7O17P3.4C6H13N/c22-17-12-19(25-7-24-17)28(8-26-12)21-16(44-46(33,34)35)14(30)11(43-21)6-41-48(38,39)45-47(36,37)40-5-10-13(29)15(31)20(42-10)27-3-1-2-9(4-27)18(23)32;4*7-6-4-2-1-3-5-6/h1,3-4,7-8,10-11,13-16,20-21,29-31H,2,5-6H2,(H2,23,32)(H,36,37)(H,38,39)(H2,22,24,25)(H2,33,34,35);4*6H,1-5,7H2/t10-,11-,13-,14-,15-,16-,20-,21-;;;/m1..../s1
InChI Key	PTKRUDMLGIORX-ITGWJZMWSA-N
SMILES string	C1CCC(CC1)N.C1CCC(CC1)N.C1CCC(CC1)N.C1CCC(CC1)N.C1C=CN(C=C1C(=O)N)[C@H]2[C@@H]([C@@H]([C@H]([C@H](O2)COP(=O)(O)OP(=O)(O)OC[C@H]3[C@H]([C@H]([C@H]([C@H](O3)N4C=NC5=C(N=CN=C54)N)OP(=O)(O)O)O)O)O)O



Form	Solid
Purity	≥98.0%, determined by LC-MS.
Solubility	Water: ≥100 mg/mL (87.56 mM); DMSO: ≥84 mg/mL (73.55 mM)
Identity	Confirmed by NMR and LC-MS.
Quality Level	Research grade
Applications	NADPH tetracyclohexanamine can be used as a reducing agent or substrate in organic synthesis and biocatalysis reactions to assist in the study of catalytic mechanisms.
Storage	Store at 4°C.
