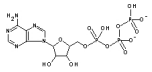

Formula: C10H14N5O13P3

MW: 505.17

Salt: 2Na+

CAS: 987-65-5

TNP NUMBER: TNP00620

MDL NUMBER: MFCD09788267

IUPAC: [5-(6-aminopurin-9-yl)-3,4-dihydroxyoxolan-2-yl]methyl hydrogen (phosphonooxy) (hydroxyphosphoryl) phosphate

Smiles: c1nc2n(C3C(O)C(O)C(O3)COP(OP(OP(=O)(O)[O-])(=O)[O-])(=O)O)cnc2c(N)n1

From Bacterial source, P2 purinergic agonist; increases activity of Ca2+-activated K+ channels; substrate for ATP-dependent enzyme systems

THERAPEUTIC CATEGORY: Coenzyme

ACCEPTORS: 13

DONORS: 6

ROTATION BONDS: 9

N+O: 18

Chiral Centers: 4

LogP: -10.02

LogS: -0.47

LIPINSKI: 1

Synonyms: adenosine-5-triphosphatedisodiumsigmagrade;Disodiumadenosine5