



Formula: C<sub>20</sub>H<sub>22</sub>N<sub>8</sub>O<sub>24</sub>P<sub>5</sub>

MW: 913.3

Salt: 5Na<sup>+</sup>, xH<sub>2</sub>O

IUPAC: [(3S,2R,4R,5R)-3,4-dihydroxy-5-(6-oxohydropurin-9-yl)oxolan-2-yl]methyl {[({[(2S,4S,5S,3R)-3,4-dihydroxy-5-(6-oxohydropurin-9-yl)oxolan-2-yl]methyl}phosphinyloxy)(hydroxyphosphoryl)]phosphinyloxy}(hydroxyphosphoryl) hydrogen phosphate

Smiles:

c1n(c2nc[nH]c(c2n1)=O)[C@H]1[C@@H]([C@@H]([C@H](COP([O-])(OP([O-])(OP(OP(OC[C@H]2[C@@H]([C@H](O)[C@H](O2)n2c3c(c([nH]cn3)=O)nc2)O)(=O)[O-])(=O)[O-])(=O)[O-])=O)O1)O)O

ACCEPTORS: 24

DONORS: 6

ROTATION BONDS: 2

N+O: 32

Chiral Centers: 8

LogP: -18.02

LogS: 0.26

LIPINSKI: 1

