Triazolo[4,5-d]pyrimidin-7-ol,3h-v-, 5-amino-3-(2',3'-o-isopropylidene-beta-d-ribofuran 5'-diphenyl phosphate (keto form)

Inchi: InChI=1S/C24H25N6O8P/c1-24(2)35-18-16(34-22(19(18)36-24)30-20-17(28-29-30)21(31
InchiKey: DUOGXSUXPRAINM-UHFFFAOYSA-N
Formula: C24H25N6O8P
SMILES: CC1(C)OC2C(COP(=O)(Oc3ccccc3)Oc3ccccc3)OC(n3nnc4c(O)nc(N)nc43)C2O1
Mol. weight [g/mol]: 556.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.80		Crippen Method
logp	3.209		Crippen Method
mcvol	368.160	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=B6008732&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume