9H-purine, 2-amino-6-methyl-9-beta-d-ribofuranosyl-

Inchi: InChI=1S/C11H15N5O4/c1-4-6-9(15-11(12)14-4)16(3-13-6)10-8(19)7(18)5(2-17)20-10/h3

InchiKey: JHXGWEHJKJZKOJ-UHFFFAOYSA-N

Formula: C11H15N5O4

SMILES: Cc1nc(N)nc2c1ncn2C1OC(CO)C(O)C1O

Mol. weight [g/mol]: 281.27

CAS: 80681-62-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.77		Crippen Method
logp	-1.672		Crippen Method
mcvol	189.450	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C80681625&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume