9H-purine, 6-amino-2-(methylamino)-9-beta-d-ribofuranosyl-

Inchi: InChI=1S/C11H16N6O4/c1-13-11-15-8(12)5-9(16-11)17(3-14-5)10-7(20)6(19)4(2-18)21-

InchiKey: UZWXAPMSNDKDNK-UHFFFAOYSA-N

Formula: C11H16N6O4

SMILES: CN=c1nc2c(ncn2C2OC(CO)C(O)C2O)c(N)[nH]1

Mol. weight [g/mol]: 296.28

CAS: 13364-95-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.40		Crippen Method
logp	-2.998		Crippen Method
mcvol	199.430	ml/mol	McGowan Method

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13364959&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume