9H-purine, 2-chloro-9-(beta-d-ribofuranosyl)-

Inchi: InChI=1S/C10H11ClN4O4/c11-10-12-1-4-8(14-10)15(3-13-4)9-7(18)6(17)5(2-16)19-9/h1
InchiKey: DXGGYSNDZSUEHC-UHFFFAOYSA-N
Formula: C10H11ClN4O4
SMILES: OCC1OC(n2cnc3cnc(Cl)nc32)C(O)C1O
Mol. weight [g/mol]: 286.67
CAS: 5466-11-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.34		Crippen Method
logp	-0.909		Crippen Method
mcvol	177.620	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=C5466115&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