

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

Inchi:	InChI=1S/C10H11CIN4O4/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:	C10H11CIN4O4
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/ci9903071
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

Latest version available from:

<https://www.chemeo.com/cid/41-817-9/9H-purine-2-chloro-9-beta-d-ribofuranosyl.pdf>

Generated by Cheméo on 2024-04-23 11:10:37.868755114 +0000 UTC m=+16159886.789332429.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.