

# 9H-purine, 6-chloro-9-(beta-d-ribofuranosyl)-

<b>Other names:</b>	6-chloro-9-«beta»-D-ribofuranosyl-9H-purine
<b>Inchi:</b>	InChI=1S/C10H11ClN4O4/c11-8-5-9(13-2-12-8)15(3-14-5)10-7(18)6(17)4(1-16)19-10/h2
<b>InchiKey:</b>	XHRJGHCQQPETRH-UHFFFAOYSA-N
<b>Formula:</b>	C10H11ClN4O4
<b>SMILES:</b>	OCC1OC(n2cnc3c(Cl)ncnc32)C(O)C1O
<b>Mol. weight [g/mol]:</b>	286.67
<b>CAS:</b>	5399-87-1

## 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

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C5399871&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5399871&amp;Units=SI</a>

## Legend

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

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