

# 9H-purine, 6-chloro-9-(2',3'-o-isopropylidene-beta-d-ribofuranosyl)-

<b>Inchi:</b>	InChI=1S/C13H15ClN4O4/c1-13(2)21-8-6(3-19)20-12(9(8)22-13)18-5-17-7-10(14)15-4-1
<b>InchiKey:</b>	VDYNZOUPLVQLRV-UHFFFAOYSA-N
<b>Formula:</b>	C13H15ClN4O4
<b>SMILES:</b>	CC1(C)OC2C(CO)OC(n3cnc4c(Cl)ncnc43)C2O1
<b>Mol. weight [g/mol]:</b>	326.74
<b>CAS:</b>	39824-26-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.75		Crippen Method
logp	0.889		Crippen Method
mcvol	209.030	ml/mol	McGowan Method

## Sources

<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=C39824265&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C39824265&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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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