

# 9H-purine-6(1h)-thione, 9-beta-d-ribofuranosyl-, 3',5'-cyclic phosphate

<b>Inchi:</b>	InChI=1S/C10H11N4O6PS/c15-6-7-4(1-18-21(16,17)20-7)19-10(6)14-3-13-5-8(14)11-2-
<b>InchiKey:</b>	JTFLPNUVMQRDAX-UHFFFAOYSA-N
<b>Formula:</b>	C10H11N4O6PS
<b>SMILES:</b>	O=P1(O)OCC2OC(n3cnc4c(=S)[nH]cnc43)C(O)C2O1
<b>Mol. weight [g/mol]:</b>	346.26
<b>CAS:</b>	20096-88-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.03		Crippen Method
logp	-0.219		Crippen Method
mcvol	203.070	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=C20096882&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C20096882&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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