

# 9H-purine, 9-methyl

<b>Inchi:</b>	InChI=1S/C6H6N4/c1-10-4-9-5-2-7-3-8-6(5)10/h2-4H,1H3
<b>InchiKey:</b>	VRZWCYZJGUYTKU-UHFFFAOYSA-N
<b>Formula:</b>	C6H6N4
<b>SMILES:</b>	Cn1cnc2cncnc21
<b>Mol. weight [g/mol]:</b>	134.14
<b>CAS:</b>	20427-22-9

## Physical Properties

Property code	Value	Unit	Source
ie	9.40	eV	NIST Webbook
log10ws	-3.86		Crippen Method
logp	0.363		Crippen Method
mcvol	96.400	ml/mol	McGowan Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C20427229&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C20427229&amp;Units=SI</a>
<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>

## Legend

<b>ie:</b>	Ionization energy
<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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