

7-Methylguanine

Other names:	6H-Purin-6-one, 2-amino-1,7-dihydro-7-methyl-Guanine, 7-methyl-N7-Methylguanine 2-Amino-7-methylhypoxanthine 2-Amino-1,7-dihydro-7-methyl-6H-purin-6-one 2-Amino-7-methyl-1,7-dihydro-6H-purin-6-one NSC 193444
Inchi:	InChI=1S/C6H7N5O/c1-11-2-8-4-3(11)5(12)10-6(7)9-4/h2H,1H3,(H3,7,9,10,12)
InchiKey:	FZWGECJQACGGTI-UHFFFAOYSA-N
Formula:	C6H7N5O
SMILES:	<chem>Cn1cnc2[nH]c(N)nc(=O)c21</chem>
Mol. weight [g/mol]:	165.15
CAS:	578-76-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.37		Crippen Method
logp	-1.243		Crippen Method
mcpol	112.250	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C578767&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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