6-Amino-1-methylpurine

Other names:	1H-Purin-6-amine, 1-methyl- Adenine, 1-methyl- 6H-Purin-6-imine, 1,9-dihydro-1-methyl- 1-methyladenine
Inchi:	InChI=1S/C6H7N5/c1-11-3-10-6-4(5(11)7)8-2-9-6/h2-3H,7H2,1H3
InchiKey:	HPZMWTNATZPBIH-UHFFFAOYSA-N
Formula:	C6H7N5
SMILES:	Cn1cnc2ncnc-2c1N
Mol. weight [g/mol]:	149.15
CAS:	5142-22-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.71		Crippen Method
logp	-0.103		Crippen Method
mcvol	106.380	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C5142223&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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