

6-Amino-3-methylpurine

Other names:	3H-Purin-6-amine, 3-methyl-Adenine, 3-methyl-3-Methyladenine 3-methyl-3H-adenine
Inchi:	InChI=1S/C6H7N5/c1-11-3-10-5(7)4-6(11)9-2-8-4/h2-3H,7H2,1H3
InchiKey:	FSASIHFSFGAIJM-UHFFFAOYSA-N
Formula:	C6H7N5
SMILES:	Cn1cnc(N)c2ncnc1-2
Mol. weight [g/mol]:	149.15
CAS:	5142-23-4

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:	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=C5142234&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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