

Purine, 2-amino-6-methylamino-

Inchi:	InChI=1S/C6H8N6/c1-8-4-3-5(10-2-9-3)12-6(7)11-4/h2H,1H3,(H4,7,8,9,10,11,12)
InchiKey:	ZAOGIVYOCDXEAK-UHFFFAOYSA-N
Formula:	C6H8N6
SMILES:	CNc1nc(N)nc2nc[nH]c12
Mol. weight [g/mol]:	164.17
CAS:	4421-04-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.44		Crippen Method
logp	-0.505		Crippen Method
mcvol	116.360	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=C4421049&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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<https://www.chemeo.com/cid/18-470-0/Purine-2-amino-6-methylamino.pdf>

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