

Purine, 2-amino-6-methyl-

Other names:	6-methyl-1H-purin-2-amine
Inchi:	InChI=1S/C6H7N5/c1-3-4-5(9-2-8-4)11-6(7)10-3/h2H,1H3,(H3,7,8,9,10,11)
InchiKey:	AFWWNHLDHNSVSD-UHFFFAOYSA-N
Formula:	C6H7N5
SMILES:	Cc1nc(N)nc2nc[nH]c12
Mol. weight [g/mol]:	149.15
CAS:	1681-10-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.90		Crippen Method
logp	-0.238		Crippen Method
mcvol	106.380	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1681103&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/21-195-2/Purine-2-amino-6-methyl.pdf>

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