

Purine, 6-chloro-8-methyl-

Inchi:	InChI=1S/C6H5ClN4/c1-3-10-4-5(7)8-2-9-6(4)11-3/h2H,1H3,(H,8,9,10,11)
InchiKey:	MZYQXIIORWCBHF-UHFFFAOYSA-N
Formula:	C6H5ClN4
SMILES:	Cc1nc2ncnc(Cl)c2[nH]1
Mol. weight [g/mol]:	168.58
CAS:	92001-52-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.95		Crippen Method
logp	0.833		Crippen Method
mcvol	108.640	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92001520&Units=SI
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

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/17-915-7/Purine-6-chloro-8-methyl.pdf>

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