

2-Chloro-6-dimethylaminopurine

Inchi:	InChI=1S/C7H8ClN5/c1-13(2)6-4-5(10-3-9-4)11-7(8)12-6/h3H,1-2H3,(H,9,10,11,12)
InchiKey:	BJAYANZFQNNNDV-UHFFFAOYSA-N
Formula:	C7H8ClN5
SMILES:	CN(C)c1nc(Cl)nc2nc[nH]c12
Mol. weight [g/mol]:	197.62
CAS:	100960-20-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.39		Crippen Method
logp	0.590		Crippen Method
mcvol	132.710	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=C100960201&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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