

Purine, 2-chloro-6-hydrazino-

Inchi:	InChI=1S/C5H5ClN6/c6-5-10-3-2(8-1-9-3)4(11-5)12-7/h1H,7H2,(H2,8,9,10,11,12)
InchiKey:	QCFNQRYMMJROEN-UHFFFAOYSA-N
Formula:	C5H5ClN6
SMILES:	NNc1nc(Cl)nc2nc[nH]c12
Mol. weight [g/mol]:	184.59
CAS:	5404-88-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.49		Crippen Method
logp	-0.190		Crippen Method
mcvol	114.510	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=C5404886&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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/67-902-6/Purine-2-chloro-6-hydrazino.pdf>

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