

5-Pyrimidinamine, 4-chloro-6-formylhydrazino-

Inchi:	InChI=1S/C5H6ClN5O/c6-4-3(7)5(9-1-8-4)11-10-2-12/h1-2H,7H2,(H,10,12)(H,8,9,11)
InchiKey:	LQZGIHUXJKFQDZ-UHFFFAOYSA-N
Formula:	C5H6ClN5O
SMILES:	<chem>Nc1c(Cl)ncnc1NNC=O</chem>
Mol. weight [g/mol]:	187.59
CAS:	89182-26-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.29		Crippen Method
logp	-0.215		Crippen Method
mcvol	121.260	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=C89182263&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/115-790-7/5-Pyrimidinamine-4-chloro-6-formylhydrazino.pdf>

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