

# Formamide, n-(4-amino-6-chloro-5-pyrimidinyl)-n-cyclopentyl-

Other names:	Formamide, n-cyclopentyl-n-(4-amino-6-chloro-5-pyrimidinyl)-
Inchi:	InChI=1S/C10H13ClN4O/c11-9-8(10(12)14-5-13-9)15(6-16)7-3-1-2-4-7/h5-7H,1-4H2,(H2
InchiKey:	FZWKJECFULLCEC-UHFFFAOYSA-N
Formula:	C10H13ClN4O
SMILES:	<chem>Nc1ncnc(Cl)c1N(C=O)C1CCCC1</chem>
Mol. weight [g/mol]:	240.69
CAS:	40067-41-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.69		Crippen Method
logp	1.618		Crippen Method
mcvol	170.870	ml/mol	McGowan Method

## Sources

NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C40067412&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C40067412&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

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

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