

# Formamide, n-(2,4-diamino-6-chloro-5-pyrimidinyl)-

Inchi:	InChI=1S/C5H6ClN5O/c6-3-2(9-1-12)4(7)11-5(8)10-3/h1H,(H,9,12)(H4,7,8,10,11)
InchiKey:	RGVJJXOLJPTHNO-UHFFFAOYSA-N
Formula:	C5H6ClN5O
SMILES:	Nc1nc(N)c(NC=O)c(Cl)n1
Mol. weight [g/mol]:	187.59
CAS:	171887-09-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.74		Crippen Method
logp	-0.137		Crippen Method
mcvol	121.260	ml/mol	McGowan Method

## Sources

NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C171887095&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C171887095&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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