

Formamide, n-(4-amino-2-chloro-5-pyrimidinyl)-

Inchi:	InChI=1S/C5H5ClN4O/c6-5-8-1-3(9-2-11)4(7)10-5/h1-2H,(H,9,11)(H2,7,8,10)
InchiKey:	IVHDXSNZTNNPRF-UHFFFAOYSA-N
Formula:	C5H5ClN4O
SMILES:	<chem>Nc1nc(Cl)ncc1NC=O</chem>
Mol. weight [g/mol]:	172.57
CAS:	116434-76-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.11		Crippen Method
logp	0.281		Crippen Method
mcvol	111.280	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=C116434765&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

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