

Formamide, n-(4-amino-2,6-dichloro-5-pyrimidinyl)-

Inchi:	InChI=1S/C5H4Cl2N4O/c6-3-2(9-1-12)4(8)11-5(7)10-3/h1H,(H,9,12)(H2,8,10,11)
InchiKey:	IWCBBJNGJRFKGT-UHFFFAOYSA-N
Formula:	C5H4Cl2N4O
SMILES:	N=c1[nH]c(Cl)nc(Cl)c1N=CO
Mol. weight [g/mol]:	207.02
CAS:	89284-45-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.79		Crippen Method
logp	0.932		Crippen Method
mcvol	123.520	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=C89284457&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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