

Formamide, n-(4-amino-2,6-dichloropyrimidin-5-yl)-n-benzyl-

Inchi:	InChI=1S/C12H10Cl2N4O/c13-10-9(11(15)17-12(14)16-10)18(7-19)6-8-4-2-1-3-5-8/h1-5
InchiKey:	ZIFCEMQHLFVMLJ-UHFFFAOYSA-N
Formula:	C12H10Cl2N4O
SMILES:	N=c1[nH]c(Cl)nc(Cl)c1N(C=O)Cc1ccccc1
Mol. weight [g/mol]:	297.14
CAS:	91962-06-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.61		Crippen Method
logp	1.877		Crippen Method
mcvol	198.390	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=C91962060&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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