

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

Inchi:	InChI=1S/C12H11ClN4O/c13-11-10(12(14)16-7-15-11)17(8-18)6-9-4-2-1-3-5-9/h1-5,7-8H
InchiKey:	CXZJQOQASZQWBV-UHFFFAOYSA-N
Formula:	C12H11ClN4O
SMILES:	<chem>N=c1[nH]cnc(Cl)c1N(C=O)Cc1ccccc1</chem>
Mol. weight [g/mol]:	262.69
CAS:	91398-41-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.93		Crippen Method
logp	1.224		Crippen Method
mcvol	186.150	ml/mol	McGowan Method

Sources

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=C91398413&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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