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