

Carbamic acid, 3-(5-amino-6-chloro-4-pyrimidinyl)-, benzyl

Inchi:
ester

InChI=1S/C12H12ClN5O2/c13-10-9(14)11(16-7-15-10)17-18-12(19)20-6-8-4-2-1-3-5-8/h

InchiKey:

VKAHDYVBDKUCMN-UHFFFAOYSA-N

Formula:

C12H12ClN5O2

SMILES:

Nc1c(Cl)ncnc1NN=C(O)OCc1ccccc1

Mol. weight [g/mol]:

293.71

CAS:

15180-19-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.42		Crippen Method
logp	2.170		Crippen Method
mcvol	202.000	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=C15180195&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

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