Formamide, n-[4-amino-6-(benzylthio)pyrimidin-5-yl]-

Inchi: InChI=1S/C12H12N4OS/c13-11-10(16-8-17)12(15-7-14-11)18-6-9-4-2-1-3-5-9/h1-5,7-8H

InchiKey: DAIXRQOOBWXPLM-UHFFFAOYSA-N

Formula: C12H12N4OS

SMILES: Nc1ncnc(SCc2ccccc2)c1N=CO

Mol. weight [g/mol]: 260.31

CAS: 91560-22-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.46		Crippen Method
logp	2.569		Crippen Method
mcvol	190.260	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=C91560224&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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