

# Formamide, n-(4-amino-6-(benzylthio)-5-pyrimidinyl)-n-ethyl-

Other names:	Pyrimidine, 4-amino-6-benzylthio-5-(n-ethylformamido)-
Inchi:	InChI=1S/C14H16N4OS/c1-2-18(10-19)12-13(15)16-9-17-14(12)20-8-11-6-4-3-5-7-11/h3
InchiKey:	GSYBXFUTYOZIHU-UHFFFAOYSA-N
Formula:	C14H16N4OS
SMILES:	CCN(C=O)c1c(N)ncnc1SCc1ccccc1
Mol. weight [g/mol]:	288.37
CAS:	92296-30-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.59		Crippen Method
logp	2.334		Crippen Method
mcvol	218.440	ml/mol	McGowan Method

## Sources

Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C92296305&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C92296305&amp;Units=SI</a>

## Legend

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

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