Formamide, n-[4-amino-6-(benzylthio)-5-pyrimidinyl]-n-benzyl-

Other names: Formamide, n-[4-amino-6-(benzylthio)pyrimidin-5-yl)]-n-benzyl-
Inchi: InChI=1S/C19H18N4OS/c20-18-17(23(14-24)11-15-7-3-1-4-8-15)19(22-13-21-18)25-12-
InchiKey: HAQQWLXTUCRJGB-UHFFFAOYSA-N
Formula: C19H18N4OS
SMILES: Nc1ncnc(SCc2ccccc2)c1N(C=O)Cc1ccccc1
Mol. weight [g/mol]: 350.44
CAS: 7461-79-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.28		Crippen Method
logp	3.514		Crippen Method
mcvol	265.130	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C7461792&Units=SI

Legend

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