

Formamide, n-(6-amino-3,4-dihydro-4-oxo-5-pyrimidinyl)-n-benzyl

Inchi: InChI=1S/C12H12N4O2/c13-11-10(12(18)15-7-14-11)16(8-17)6-9-4-2-1-3-5-9/h1-5,7-8H
InchiKey: PJPOUWBXGZIXIZ-UHFFFAOYSA-N
Formula: C12H12N4O2
SMILES: Nc1nc[nH]c(=O)c1N(C=O)Cc1ccccc1
Mol. weight [g/mol]: 244.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.31		Crippen Method
logp	0.033		Crippen Method
mcvol	179.780	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=B6009947&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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