

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

Inchi:	InChI=1S/C7H11N5O/c1-12(2)7-5(11-4-13)6(8)9-3-10-7/h3-4H,1-2H3,(H,11,13)(H2,8,9,1
InchiKey:	OLAJAXLMRSNMFK-UHFFFAOYSA-N
Formula:	C7H11N5O
SMILES:	CN(C)c1ncnc(N)c1NC=O
Mol. weight [g/mol]:	181.20
CAS:	98335-68-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.33		Crippen Method
logp	-0.307		Crippen Method
mcvol	137.200	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C98335683&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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