

4-Cyclopropyl-6-methyl-N-acetyl-N-phenylpyrimidin-2-amine

Other names:	2-Pyrimidinamine, 4-cyclopropyl-6-methyl-N-acetyl-N-phenyl-Cyprodinil acetate
Inchi:	InChI=1S/C16H17N3O/c1-11-10-15(13-8-9-13)18-16(17-11)19(12(2)20)14-6-4-3-5-7-14/
InchiKey:	YNIZVZRQLSYJKQ-UHFFFAOYSA-N
Formula:	C16H17N3O
SMILES:	CC(=O)N(c1cccc1)c1nc(C)cc(C2CC2)n1
Mol. weight [g/mol]:	267.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.46		Crippen Method
logp	3.347		Crippen Method
mcvol	209.430	ml/mol	McGowan Method
rinpol	2178.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373447&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol:	Non-polar retention indices

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