4-Cyclopropyl-6-methyl-N-acetyl-N-phenylpyrimid

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/h
InchiKey: YNIZVZRQLSYJKQ-UHFFFAOYSA-N
Formula: C16H17N3O
SMILES: CC(=O)N(c1ccccc1)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