N-(4,6-Dimethylpyrimidin-2-yl)-N-phenylacetamide

Other names: 2-Pyrimidinamine, 4,6-dimethyl-N-acetyl-N-phenyl-
4,6-Dimethyl-N-acetyl-N-phenyl-2-pyrimidinamine
N-Acetyl-N-phenyl-4,6-dimethyl-2-pyrimidinamine
4,6-Dimethyl-N-phenyl-pyrimidin-2-amine acetate
Inchi: InChI=1S/C14H15N3O/c1-10-9-11(2)16-14(15-10)17(12(3)18)13-7-5-4-6-8-13/h4-9H,1-3
InchiKey: RWIQLYHYUNCBSK-UHFFFAOYSA-N
Formula: C14H15N3O
SMILES: CC(=O)N(c1ccccc1)c1nc(C)cc(C)n1
Mol. weight [g/mol]: 241.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.85		Crippen Method
logp	2.778		Crippen Method
mcvol	192.110	ml/mol	McGowan Method
rinpol	1957.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373335&Units=SI
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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices