2-Pyrimidinamine, 4,6-dimethyl-N-trifluoroacetyl-N-phenyl-

Other names: 4,6-Dimethyl-N-phenyl-N-trifluoroacetyl-2-pyrimidinamine
4,6-Dimethyl-N-phenyl-N-trifluoroacetylpyrimidin-2-amine
N-Phenyl-N-trifluoroacetyl-4,6-dimethyl-2-pyrimidinamine
N-(4,6-dimethylpyrimidin-2-yl)-2,2,2-trifluoro-N-phenylacetamide

Inchi: InChI=1S/C14H12F3N3O/c1-9-8-10(2)19-13(18-9)20(12(21)14(15,16)17)11-6-4-3-5-7-11

InchiKey: VEALWEQKPWFQGS-UHFFFAOYSA-N

Formula: C14H12F3N3O

SMILES: Cc1cc(C)nc(N(C(=O)C(F)(F)F)c2ccccc2)n1

Mol. weight [g/mol]: 295.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.52		Crippen Method
logp	3.320		Crippen Method
mcvol	197.420	ml/mol	McGowan Method
rinpol	1734.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373317&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices