4-Cyclopropyl-6-methyl-N-phenyl-N-trifluoroacety

Other names: 2-Pyrimidinamine, 4-cyclopropyl-6-methyl-N-phenyl-N-trifluoroacetyl-
4-Cyclopropyl-6-methyl-N-phenyl-N-trifluoroacetyl-2-pyrimidinamine
Cyprodinil trifluoroacetate
Inchi: InChI=1S/C16H14F3N3O/c1-10-9-13(11-7-8-11)21-15(20-10)22(14(23)16(17,18)19)12-5
InchiKey: YMHCSDPMOKIOIK-UHFFFAOYSA-N
Formula: C16H14F3N3O
SMILES: Cc1cc(C2CC2)nc(N(C(=O)C(F)(F)F)c2ccccc2)n1
Mol. weight [g/mol]: 321.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.12		Crippen Method
logp	3.889		Crippen Method
mcvol	214.740	ml/mol	McGowan Method
rinpol	1940.00		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=U372984&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

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