

4-Cyclopropyl-6-methyl-N-phenyl-N-trifluoroacetyl

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:	YMHCS DPMOKIOIK-UHFFFAOYSA-N
Formula:	C16H14F3N3O
SMILES:	<chem>Cc1cc(C2CC2)nc(N(C(=O)C(F)(F)F)c2ccccc2)n1</chem>
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/ci9903071
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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