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

Other names: 4,6-Dimethyl-N-pentafluoropropionyl-N-phenyl-2-pyrimidinamine
Inchi: InChI=1S/C15H12F5N3O/c1-9-8-10(2)22-13(21-9)23(11-6-4-3-5-7-11)12(24)14(16,17)15
InchiKey: DLJMRZHECVMFKA-UHFFFAOYSA-N
Formula: C15H12F5N3O
SMILES: Cc1cc(C)nc(N(C(=O)C(F)(F)C(F)(F)F)c2ccccc2)n1
Mol. weight [g/mol]: 345.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.25		Crippen Method
logp	3.956		Crippen Method
mcvol	215.050	ml/mol	McGowan Method
rinpol	1701.00		NIST Webbook

Sources

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=U373090&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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