

1,5,6-Triazabicyclo[3.1.0]hexane, 4-methyl-2,2,6-tris(trifluoromethyl)-4-phenyl-

Inchi: InChI=1S/C13H10F9N3/c1-9(8-5-3-2-4-6-8)7-10(11(14,15)16,12(17,18)19)24-23(9)25(24)
InchiKey: PTIRVBOPZPHAQT-UHFFFAOYSA-N
Formula: C13H10F9N3
SMILES: CC1(c2ccccc2)CC(C(F)(F)F)(C(F)(F)F)n2n(C(F)(F)F)n21
Mol. weight [g/mol]: 379.22
CAS: 95388-88-8

Physical Properties

Property code	Value	Unit	Source
ie	9.00	eV	NIST Webbook
ie	9.30	eV	NIST Webbook
log10ws	-5.68		Crippen Method
logp	4.554		Crippen Method
mcvol	194.420	ml/mol	McGowan Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C95388888&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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