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

Inchi: InChI=1S/C8H8F9N3/c1-4(2)3-5(6(9,10)11,7(12,13)14)19-18(4)20(19)8(15,16)17/h3H2,1
InchiKey: IYRJFKPSRCNEOA-UHFFFAOYSA-N
Formula: C8H8F9N3
SMILES: CC1(C)CC(C(F)(F)F)(C(F)(F)F)n2n(C(F)(F)F)n21
Mol. weight [g/mol]: 317.15
CAS: 95388-86-6

Physical Properties

Property code	Value	Unit	Source
ie	10.00	eV	NIST Webbook
ie	10.65	eV	NIST Webbook
log10ws	-4.38		Crippen Method
logp	3.526		Crippen Method
mcvol	147.730	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=C95388866&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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