Spirocyclopentane-2-(1,5,6-triazabicyclo[3.1.0]hex-4,4,6-tris(trifluoromethyl)-

InChI: InChI=1S/C10H10F9N3/c11-8(12,13)7(9(14,15)16)5-6(3-1-2-4-6)20-21(7)22(20)10(17,18

InChIKey: WAUKETKYWVDCAK-UHFFFAOYSA-N

Formula: C10H10F9N3

SMILES: FC(F)(F)n1n2n1C(C(F)(F)F)(C(F)(F)F)CC21CCCC1

Mol. weight [g/mol]: 343.19

CAS: 130720-66-0

Physical Properties

Property code	Value	Unit	Source
ie	10.00	eV	NIST Webbook
ie	10.43	eV	NIST Webbook
log10ws	-5.11		Crippen Method
logp	4.060		Crippen Method
mcvol	165.050	ml/mol	McGowan Method

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=C130720660&Units=SI

Legend

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume