

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/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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