

# Spirocyclohexane-2-(1,5,6-triazabicyclo[3.1.0]hexane-4,4,6-tris(trifluoromethyl)-

InchiKey: BNSGZLXKEANLBR-UHFFFAOYSA-N  
Mol. Weight: 357.22

**Formula:** C<sub>11</sub>H<sub>12</sub>F<sub>9</sub>N<sub>3</sub>  
**SMILES:** FC(F)(F)n1n2n1C(C(F)(F)F)(C(F)(F)F)CC21CCCCC1  
**Mol. weight [g/mol]:** 357.22  
**CAS:** 130720-67-1

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| ie            | 9.70    | eV     | NIST Webbook   |
| ie            | 10.41   | eV     | NIST Webbook   |
| log10ws       | -5.53   |        | Crippen Method |
| logp          | 4.450   |        | Crippen Method |
| mcvol         | 179.140 | ml/mol | McGowan Method |

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=C130720671&Units=SI>

## 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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