

# 2,2,2-Trifluoro-N-(6-Methoxy-1,3-benzothiazol-2-yl)

**Inchi:** InChI=1S/C10H7F3N2O2S/c1-17-5-2-3-6-7(4-5)18-9(14-6)15-8(16)10(11,12)13/h2-4H,1H  
**InchiKey:** WSJVIIIZYSKITEU-UHFFFAOYSA-N  
**Formula:** C10H7F3N2O2S  
**SMILES:** COc1ccc2nc(NC(=O)C(F)(F)F)sc2c1  
**Mol. weight [g/mol]:** 276.24

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.78		Crippen Method
logp	2.806		Crippen Method
mcvol	161.900	ml/mol	McGowan Method
rinpol	1858.00		NIST Webbook
rinpol	1858.00		NIST Webbook

## Sources

**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=U373106&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices

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