N-(5,6-Dichloro-1,3-benzothiazol-2-yl)-2,2,3,3,3-pe

Inchi: InChI=1S/C10H3Cl2F5N2OS/c11-3-1-5-6(2-4(3)12)21-8(18-5)19-7(20)9(13,14)10(15,16)
InchiKey: YRTUNOSCVKICLA-UHFFFAOYSA-N
Formula: C10H3Cl2F5N2OS
SMILES: O=C(Nc1nc2cc(Cl)c(Cl)cc2s1)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 365.11

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.77		Crippen Method
logp	4.739		Crippen Method
mcvol	184.050	ml/mol	McGowan Method
rinpol	1938.00		NIST Webbook

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=U373454&Units=SI

Legend

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