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

Inchi: InChI=1S/C9H3Cl2F3N2OS/c10-3-1-5-6(2-4(3)11)18-8(15-5)16-7(17)9(12,13)14/h1-2H,(
InchiKey: WKYNHNRROJBZCK-UHFFFAOYSA-N
Formula: C9H3Cl2F3N2OS
SMILES: OC(=Nc1nc2cc(Cl)c(Cl)cc2s1)C(F)(F)F
Mol. weight [g/mol]: 315.10

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.22		Crippen Method
logp	4.753		Crippen Method
mcvol	166.420	ml/mol	McGowan Method
rinpol	1954.00		NIST Webbook
rinpol	1954.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373290&Units=SI
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

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.