N-(5,6-Dichloro-1,3-benzothiazol-2-yl)-2,2,3,3,4,4,4

Inchi: InChI=1S/C11H3Cl2F7N2OS/c12-3-1-5-6(2-4(3)13)24-8(21-5)22-7(23)9(14,15)10(16,17)
InchiKey: DVLQZIJQEZEOEN-UHFFFAOYSA-N
Formula: C11H3Cl2F7N2OS
SMILES: O=C(Nc1nc2cc(Cl)c(Cl)cc2s1)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 415.11

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.50		Crippen Method
logp	5.375		Crippen Method
mcvol	201.680	ml/mol	McGowan Method
rinpol	1972.00		NIST Webbook
rinpol	1972.00		NIST Webbook

Sources

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=U373289&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

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