N-(6-Methoxy-1,3-benzothiazol-2-yl)-2,2,3,3,4,4,4-h

Inchi: InChI=1S/C12H7F7N2O2S/c1-23-5-2-3-6-7(4-5)24-9(20-6)21-8(22)10(13,14)11(15,16)12
InchiKey: DGVLJTVBRPRXAL-UHFFFAOYSA-N
Formula: C12H7F7N2O2S
SMILES: COc1ccc2nc(NC(=O)C(F)(F)C(F)(F)C(F)(F)F)sc2c1
Mol. weight [g/mol]: 376.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.25		Crippen Method
logp	4.076		Crippen Method
mcvol	197.160	ml/mol	McGowan Method
rinpol	1882.00		NIST Webbook
rinpol	1882.00		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=U373217&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

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