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

Inchi: InChI=1S/C11H7F5N2O2S/c1-20-5-2-3-6-7(4-5)21-9(17-6)18-8(19)10(12,13)11(14,15)16
InchiKey: KEHJSZHTCSEWGG-UHFFFAOYSA-N
Formula: C11H7F5N2O2S
SMILES: COc1ccc2nc(NC(=O)C(F)(F)C(F)(F)F)sc2c1
Mol. weight [g/mol]: 326.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.52		Crippen Method
logp	3.441		Crippen Method
mcvol	179.530	ml/mol	McGowan Method
rinpol	1848.00		NIST Webbook
rinpol	1848.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373216&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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.