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

Other names: 4-Methoxy-1,3-benzothiazol-2-amine, N,N-bis(pentafluoropropionyl)-
Inchi: InChI=1S/C14H6F10N2O3S/c1-29-5-3-2-4-6-7(5)25-10(30-6)26(8(27)11(15,16)13(19,20)
InchiKey: ROBKCRVADXHVCW-UHFFFAOYSA-N
Formula: C14H6F10N2O3S
SMILES: COc1cccc2sc(N(C(=O)C(F)(F)C(F)(F)F)C(=O)C(F)(F)C(F)(F)F)nc12
Mol. weight [g/mol]: 472.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.00		Crippen Method
logp	4.560		Crippen Method
mcvol	232.220	ml/mol	McGowan Method
rinpol	1919.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373333&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

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