2,2,2-Trifluoro-N-(4-methoxy-1,3-benzothiazol-2-yl

Inchi: InChI=1S/C10H7F3N2O2S/c1-17-5-3-2-4-6-7(5)14-9(18-6)15-8(16)10(11,12)13/h2-4H,1H

InchiKey: FIFSMPPVRLCFOT-UHFFFAOYSA-N

Formula: C10H7F3N2O2S

SMILES: COc1cccc2sc(NC(=O)C(F)(F)F)nc12

Mol. weight [g/mol]: 276.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.78		Crippen Method
logp	2.806		Crippen Method
mcvol	161.900	ml/mol	McGowan Method
rinpol	1950.00		NIST Webbook
rinpol	1950.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373113&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.