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

Inchi: InChI=1S/C10H10N2O2S/c1-6(13)11-10-12-9-7(14-2)4-3-5-8(9)15-10/h3-5H,1-2H3,(H,11
InchiKey: AQDZPXNDPBKKSZ-UHFFFAOYSA-N
Formula: C10H10N2O2S
SMILES: COc1cccc2sc(NC(C)=O)nc12
Mol. weight [g/mol]: 222.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.12		Crippen Method
logp	2.263		Crippen Method
mcvol	156.590	ml/mol	McGowan Method
rinpol	2254.00		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=U373134&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