Thiazolidine, N-isoBOC

Inchi: InChI=1S/C8H15NO2S/c1-7(2)5-11-8(10)9-3-4-12-6-9/h7H,3-6H2,1-2H3
InchiKey: GHXFPPIBOBSDAR-UHFFFAOYSA-N
Formula: C8H15NO2S
SMILES: CC(C)COC(=O)N1CCSC1
Mol. weight [g/mol]: 189.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.61		Crippen Method
logp	1.785		Crippen Method
mcvol	146.490	ml/mol	McGowan Method
rinpol	1476.00		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=R392860&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

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