Zolimidine

Inchi: InChI=1S/C14H12N2O2S/c1-19(17,18)12-7-5-11(6-8-12)13-10-16-9-3-2-4-14(16)15-13/h
InchiKey: VSLIUWLPFRVCDL-UHFFFAOYSA-N
Formula: C14H12N2O2S
SMILES: CS(=O)(=O)c1ccc(-c2cn3ccccc3n2)cc1
Mol. weight [g/mol]: 272.32
CAS: 1222-57-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.49		Crippen Method
logp	2.405		Crippen Method
mcvol	193.490	ml/mol	McGowan Method
rinpol	2927.00		NIST Webbook
rinpol	2927.00		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=C1222577&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