3-((Methylsulfonyl)methyl)-1H-indole

Inchi: InChI=1S/C10H11NO2S/c1-14(12,13)7-8-6-11-10-5-3-2-4-9(8)10/h2-6,11H,7H2,1H3
InchiKey: QLXXKTRCCMXQTL-UHFFFAOYSA-N
Formula: C10H11NO2S
SMILES: CS(=O)(=O)Cc1c[nH]c2ccccc12
Mol. weight [g/mol]: 209.26
CAS: 857775-86-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.63		Crippen Method
logp	1.231		Crippen Method
mcvol	150.910	ml/mol	McGowan Method
rinpol	2242.50		NIST Webbook
rinpol	2242.50		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=C857775861&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