1-[3-(Dimethylamino)propyl]indole

Other names: N,N-dimethyl-1H-indole-1-propylamine
Inchi: InChI=1S/C13H18N2/c1-14(2)9-5-10-15-11-8-12-6-3-4-7-13(12)15/h3-4,6-8,11H,5,9-10H
InchiKey: VZQZKEYQPBNATK-UHFFFAOYSA-N
Formula: C13H18N2
SMILES: CN(C)CCCn1ccc2ccccc21
Mol. weight [g/mol]: 202.30
CAS: 20892-46-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.36		Crippen Method
logp	2.593		Crippen Method
mcvol	175.070	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20892460&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