1-(3-Indolyl)-1-propanone

Other names: 1-(1H-indol-3-yl)propan-1-one
Inchi: InChI=1S/C11H11NO/c1-2-11(13)9-7-12-10-6-4-3-5-8(9)10/h3-7,12H,2H2,1H3
InchiKey: KMVYYLYKRGELJE-UHFFFAOYSA-N
Formula: C11H11NO
SMILES: CCC(=O)c1c[nH]c2ccccc12
Mol. weight [g/mol]: 173.21
CAS: 22582-68-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.57		Crippen Method
logp	2.279		Crippen Method
mcvol	138.480	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C22582689&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume