1H-Indol-3-amine

Inchi: InChI=1S/C8H8N2/c9-7-5-10-8-4-2-1-3-6(7)8/h1-5,10H,9H2
InchiKey: TXQAZWIBPGKHOX-UHFFFAOYSA-N
Formula: C8H8N2
SMILES: Nc1c[nH]c2ccccc12
Mol. weight [g/mol]: 132.16
CAS: 7250-19-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.13		Crippen Method
logp	1.268		Crippen Method
mcvol	104.620	ml/mol	McGowan Method

Sources

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=C7250193&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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