

5-Hydroxyindoleacetic acid, methyl

Inchi: InChI=1S/C11H11NO3/c1-15-11(14)4-7-6-12-10-3-2-8(13)5-9(7)10/h2-3,5-6,12-13H,4H2
InchiKey: ICPIRXLDEXTULL-UHFFFAOYSA-N
Formula: C11H11NO3
SMILES: COC(=O)Cc1c[nH]c2ccc(O)cc12
Mol. weight [g/mol]: 205.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.13		Crippen Method
logp	1.107		Crippen Method
mcvol	150.220	ml/mol	McGowan Method
rinpol	2051.00		NIST Webbook
rinpol	2051.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R579978&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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
rinpol: Non-polar retention indices

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