5-Methoxy-4-methoxymethyl-2-methyl-1H-indole

Inchi: InChI=1S/C12H15NO2/c1-8-6-9-10(7-14-2)12(15-3)5-4-11(9)13-8/h4-6,13H,7H2,1-3H3
InchiKey: OQSVAFCMVCOFGM-UHFFFAOYSA-N
Formula: C12H15NO2
SMILES: COCc1c(OC)ccc2[nH]c(C)cc12
Mol. weight [g/mol]: 205.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.48		Crippen Method
logp	2.149		Crippen Method
mcvol	162.740	ml/mol	McGowan Method
rinpol	1800.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R586213&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
rinpol: Non-polar retention indices