5-Methoxy-2,4-dimethyl-1H-indole

Inchi: InChI=1S/C11H13NO/c1-7-6-9-8(2)11(13-3)5-4-10(9)12-7/h4-6,12H,1-3H3
InchiKey: GRXIPOZSDQNWRO-UHFFFAOYSA-N
Formula: C11H13NO
SMILES: COc1ccc2[nH]c(C)cc2c1C
Mol. weight [g/mol]: 175.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.57		Crippen Method
logp	2.311		Crippen Method
mcvol	142.780	ml/mol	McGowan Method
rinpol	1719.00		NIST Webbook
rinpol	1719.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R586208&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

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