Methyl 5-chloro-1H-indole-2-carboxylate

Inchi: InChI=1S/C10H8ClNO2/c1-14-10(13)9-5-6-4-7(11)2-3-8(6)12-9/h2-5,12H,1H3
InchiKey: WGAOEHZSJWVLBY-UHFFFAOYSA-N
Formula: C10H8ClNO2
SMILES: COC(=O)c1cc2cc(Cl)ccc2[nH]1
Mol. weight [g/mol]: 209.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.42		Crippen Method
logp	2.126		Crippen Method
mcvol	142.500	ml/mol	McGowan Method
rinpol	1875.00		NIST Webbook
rinpol	1875.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373011&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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