4-CHLORO-INDOLEACETIC ACID METHYL ESTER

Other names: Methyl 4-chloroindolyl-3-acetate
Inchi: InChI=1S/C11H10ClNO2/c1-15-10(14)5-7-6-13-9-4-2-3-8(12)11(7)9/h2-4,6,13H,5H2,1H3
InchiKey: SYPGJEURLIGNPE-UHFFFAOYSA-N
Formula: C11H10ClNO2
SMILES: COC(=O)Cc1c[nH]c2cccc(Cl)c12
Mol. weight [g/mol]: 223.66

Physical Properties

Property code	Value	Unit	Source
logp	2.055		Crippen Method
mcvol	156.590	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C19077782&Units=SI

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume