

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

Latest version available from:

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