

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:	<chem>COC(=O)Cc1c[nH]c2cccc(Cl)c12</chem>
Mol. weight [g/mol]:	223.66
CAS:	19077-78-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.26		Crippen Method
logp	2.055		Crippen Method
mcvol	156.590	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19077782&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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