

Indole-3-acetic acid, 6-chloro-2-methyl-

Inchi:	InChI=1S/C11H10ClNO2/c1-6-9(5-11(14)15)8-3-2-7(12)4-10(8)13-6/h2-4,13H,5H2,1H3,(
InchiKey:	CRCFIUIKYLJTBK-UHFFFAOYSA-N
Formula:	C11H10ClNO2
SMILES:	Cc1[nH]c2cc(Cl)ccc2c1CC(=O)O
Mol. weight [g/mol]:	223.66
CAS:	6127-21-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.56		Crippen Method
logp	2.275		Crippen Method
mcvol	156.590	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6127215&Units=SI
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

Legend

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

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