

n-Butyl 5-chloro-1H-indole-2-carboxylate

Other names:	1H-Indole-2-carboxylic acid, 5-chloro-, n-butyl ester
Inchi:	InChI=1S/C13H14ClNO2/c1-2-3-6-17-13(16)12-8-9-7-10(14)4-5-11(9)15-12/h4-5,7-8,15H
InchiKey:	ULGAZQRBTCPFDK-UHFFFAOYSA-N
Formula:	C13H14ClNO2
SMILES:	CCCCOC(=O)c1cc2cc(Cl)ccc2[nH]1
Mol. weight [g/mol]:	251.71

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.68		Crippen Method
logp	3.296		Crippen Method
mcvol	184.770	ml/mol	McGowan Method
rinpol	2154.00		NIST Webbook
rinpol	2154.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373012&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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