

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: ULGAZQRBTPCFDK-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
rinpola	2154.00		NIST Webbook
rinpola	2154.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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=U373012&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpola: Non-polar retention indices

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