5-Chloro-1H-indole-2-carboxylic acid, tert-butyldimethylsilyl ester

Other names: 5-Chloro-1H-indole-2-carboxylic acid, BDMS
Inchi: InChI=1S/C15H20ClNO2Si/c1-15(2,3)20(4,5)19-14(18)13-9-10-8-11(16)6-7-12(10)17-13/
InchiKey: JYUAWRCUJOPLTK-UHFFFAOYSA-N
Formula: C15H20ClNO2Si
SMILES: CC(C)(C)[Si](C)(C)OC(=O)c1cc2cc(Cl)ccc2[nH]1
Mol. weight [g/mol]: 309.86

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.57		Crippen Method
logp	4.501		Crippen Method
rinpol	2269.00		NIST Webbook
rinpol	2269.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373347&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices