

1-(tert-Butyldimethylsilyl)-5-chloroindole-2-carboxylic acid, tert-butyl dimethylsilyl ester

Other names: 5-Chloro-1H-indole-1-carboxylic acid, N,O-di-*t*BDMS
Inchi: InChI=1S/C21H34ClNO2Si2/c1-20(2,3)26(7,8)23-17-12-11-16(22)13-15(17)14-18(23)19(20,21)24-25
InchiKey: CHJGYUKTXISVOG-UHFFFAOYSA-N
Formula: C21H34ClNO2Si2
SMILES: CC(C)(C)[Si](C)(C)OC(=O)c1cc2cc(Cl)ccc2n1[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 424.12

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.94		Crippen Method
logp	7.310		Crippen Method
rinpol	2527.00		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=U373348&Units=SI>

Legend

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

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