

5-Chloro-1H-indole-2-carboxylic acid, trimethylsilyl ester

Other names: 5-Chloro-1H-indole-2-carboxylic acid TMS

Inchi: InChI=1S/C12H14ClNO2Si/c1-17(2,3)16-12(15)11-7-8-6-9(13)4-5-10(8)14-11/h4-7,14H,1

InchiKey: DVRXHLFAWBKKSS-UHFFFAOYSA-N

Formula: C₁₂H₁₄ClNO₂Si

SMILES: C[Si](C)(C)OC(=O)c1cc2cc(Cl)ccc2[nH]1

Mol. weight [g/mol]: 267.78

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	3.331		Crippen Method
rinpol	2008.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U373115&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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