

Indole-3-carboxylic acid, TMS

Inchi: InChI=1S/C15H23NO2Si2/c1-19(2,3)16-11-13(15(17)18-20(4,5)6)12-9-7-8-10-14(12)16/h
InchiKey: MUCQUVKAUPBCGI-UHFFFAOYSA-N
Formula: C15H23NO2Si2
SMILES: C[Si](C)(C)OC(=O)c1cn([Si](C)(C)C)c2ccccc12
Mol. weight [g/mol]: 305.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.74		Crippen Method
logp	4.316		Crippen Method
rinsol	1999.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R94937&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/32-224-7/Indole-3-carboxylic-acid-TMS.pdf>

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