

N-Trimethylsilylindoleacetic acid, methyl ester

Other names: IAA, MeTMS
Indole-3-acetic acid, (Me,TMS)
Methyl 3-indolylacetate, tms derivative

Inchi: InChI=1S/C14H19NO2Si/c1-17-14(16)9-11-10-15(18(2,3)4)13-8-6-5-7-12(11)13/h5-8,10H

InchiKey: OVBJETHPLUQCEW-UHFFFAOYSA-N

Formula: C14H19NO2Si

SMILES: COC(=O)Cc1cn([Si](C)(C)C)c2ccccc12

Mol. weight [g/mol]: 261.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.70		Crippen Method
logp	3.040		Crippen Method
rinpol	1860.00		NIST Webbook
rinpol	1869.00		NIST Webbook
rinpol	1853.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U101027&Units=SI>

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

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/36-123-5/N-Trimethylsilylindoleacetic-acid-methyl-ester.pdf>

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