

3-Indoleacetic acid, tert-butyldimethylsilyl ester

Other names:	3-Indoleacetic acid, tbdms derivative
Inchi:	InChI=1S/C16H23NO2Si/c1-16(2,3)20(4,5)19-15(18)10-12-11-17-14-9-7-6-8-13(12)14/h6
InchiKey:	IDZOKLIQJYIVQF-UHFFFAOYSA-N
Formula:	C16H23NO2Si
SMILES:	CC(C)(C)[Si](C)(C)OC(=O)Cc1c[nH]c2ccccc12
Mol. weight [g/mol]:	289.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.72		Crippen Method
logp	3.777		Crippen Method
rinpol	2188.60		NIST Webbook
rinpol	2188.60		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=U333993&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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<https://www.chemeo.com/cid/29-862-3/3-Indoleacetic-acid-tert-butyldimethylsilyl-ester.pdf>

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