

# 1H-Indole-3-propanoic acid, 1-(trimethylsilyl)-, trimethylsilyl ester

<b>Other names:</b>	3-Indolepropionic acid (2TMS) 3-Indole propanoic acid diTMS Indole-3-propionic acid, bis-TMS Indole-3-propionic acid, diTMS Indole-3-propionic acid, TMS 3-Indolepropionic acid, 2tms derivative
<b>Inchi:</b>	InChI=1S/C17H27NO2Si2/c1-21(2,3)18-13-14(15-9-7-8-10-16(15)18)11-12-17(19)20-22
<b>InchiKey:</b>	MMSXZNPQCUIOIS-UHFFFAOYSA-N
<b>Formula:</b>	C17H27NO2Si2
<b>SMILES:</b>	<chem>C[Si](C)(C)OC(=O)CCc1cn([Si](C)(C)C)c2ccccc12</chem>
<b>Mol. weight [g/mol]:</b>	333.57
<b>CAS:</b>	55191-57-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.00		Crippen Method
logp	4.635		Crippen Method
rinpol	2066.00		NIST Webbook
rinpol	2089.00		NIST Webbook
rinpol	2089.00		NIST Webbook
rinpol	2066.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C55191576&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C55191576&amp;Units=SI</a>

## Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**rinpol:** Non-polar retention indices

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