

1H-Indole-1-acetic acid, trimethylsilyl ester

Other names:	Indole-1-acetic acid TMS 1H-indole-1-acetic acid, tms derivative
Inchi:	InChI=1S/C13H17NO2Si/c1-17(2,3)16-13(15)10-14-9-8-11-6-4-5-7-12(11)14/h4-9H,10H2
InchiKey:	QSNYXYIMLGVIJP-UHFFFAOYSA-N
Formula:	C13H17NO2Si
SMILES:	C[Si](C)(C)OC(=O)Cn1ccc2ccccc21
Mol. weight [g/mol]:	247.37
CAS:	74367-53-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.71		Crippen Method
logp	3.019		Crippen Method
rinpol	1917.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74367536&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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<https://www.chemeo.com/cid/22-483-1/1H-Indole-1-acetic-acid-trimethylsilyl-ester.pdf>

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