

Indole-3-glycolic acid, TMS

Inchi: InChI=1S/C16H25NO3Si2/c1-21(2,3)17-11-15(13-9-7-8-10-14(13)17)19-12-16(18)20-22
InchiKey: WYLSKTRMJDOEIG-UHFFFAOYSA-N
Formula: C16H25NO3Si2
SMILES: C[Si](C)(C)OC(=O)COc1cn([Si](C)(C)C)c2ccccc12
Mol. weight [g/mol]: 335.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.32		Crippen Method
logp	4.081		Crippen Method
rinpol	2018.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R94941&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/49-904-4/Indole-3-glycolic-acid-TMS.pdf>

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