

Indole-3-lactic acid, TMS

Inchi: InChI=1S/C19H33NO3Si3/c1-24(2,3)20-14-16(15-12-10-11-13-17(15)20)18(22-25(4,5)6)
InchiKey: OPVNSBUMGPXNFG-UHFFFAOYSA-N
Formula: C19H33NO3Si3
SMILES: C[Si](C)(C)OC(=O)C(O[Si](C)(C)C)c1cn([Si](C)(C)C)c2ccccc12
Mol. weight [g/mol]: 407.73

Physical Properties

Property code	Value	Unit	Source
log10ws	0.56		Crippen Method
logp	5.595		Crippen Method
rinpol	2180.00		NIST Webbook
rinpol	2180.00		NIST Webbook
rinpol	2180.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R94955&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/114-099-6/Indole-3-lactic-acid-TMS.pdf>

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