

1H-Indole-3-acetic acid, 1-(trimethylsilyl)-5-[(trimethylsilyl)oxy]-, trimethylsilyl ester

Other names

5-Hydroxyindoleacetic acid (3TMS)
5-Hydroxyindole-3-acetic acid, tris-TMS
Indol-3-acetic acid, 5-hydroxy, (3TMS)-
Indol-3-acetic acid, 5-hydroxy, tri-TMS
Indole-3-acetic acid, 5-hydroxy, tris-TMS
Indole-3-acetic acid, 5-hydroxy, TMS
5-Hydroxyindoleacetic acid (tms)
Indol-3-acetic acid, 5-hydroxy, TMS
5-Hydroxyindole-3-acetic acid, TMS
5-Hydroxyindoleacetic acid, 3tms derivative

Inchi: InChI=1S/C19H33NO3Si3/c1-24(2,3)20-14-15(12-19(21)23-26(7,8)9)17-13-16(10-11-18)
InchiKey: RUKKQUFMPLELJQ-UHFFFAOYSA-N
Formula: C19H33NO3Si3
SMILES: C[Si](C)(C)OC(=O)Cc1cn([Si](C)(C)C)c2ccc(O[Si](C)(C)C)cc12
Mol. weight [g/mol]: 407.73
CAS: 55268-67-2

Physical Properties

Property code	Value	Unit	Source
log10ws	0.41		Crippen Method
logp	5.459		Crippen Method
rinpol	2199.00		NIST Webbook
rinpol	2239.00		NIST Webbook
rinpol	2168.00		NIST Webbook
rinpol	2200.00		NIST Webbook
rinpol	2199.00		NIST Webbook
rinpol	2249.00		NIST Webbook
rinpol	2190.00		NIST Webbook
rinpol	2249.00		NIST Webbook
rinpol	2199.00		NIST Webbook
rinpol	2204.00		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=C55268672&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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