

2-Propenoic acid, 3-[1-(trimethylsilyl)-1H-indol-3-yl]-, trimethylsilyl ester

Other names: Trimethylsilyl 3-[1-(trimethylsilyl)-1H-indol-3-yl]-2-propenoate
Indole-3-acrylic acid, N,O-bis-TMS

Indole-3-acrylic acid, TMS

Indoleacrylic acid, 2tms derivative

Inchi: InChI=1S/C17H25NO2Si2/c1-21(2,3)18-13-14(15-9-7-8-10-16(15)18)11-12-17(19)20-22

InchiKey: QGUSJWZJGZJSGS-VAWYXSNFSA-N

Formula: C17H25NO2Si2

SMILES: C[Si](C)(C)OC(=O)C=Cc1cn([Si](C)(C)C)c2ccccc12

Mol. weight [g/mol]: 331.56

CAS: 55124-88-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.02		Crippen Method
logp	4.716		Crippen Method
rinpol	2357.00		NIST Webbook
rinpol	2402.20		NIST Webbook
rinpol	2357.00		NIST Webbook
rinpol	2402.20		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=C55124884&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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