5-Hydroxyindoleacetic acid, ethoxycarbonylated, TBDMS

Inchi: InChI=1S/C25H41NO5Si2/c1-12-29-23(28)26-17-18(15-22(27)31-33(10,11)25(5,6)7)20-1

InchiKey: UKRRCJNYBUNIEU-UHFFFAOYSA-N

Formula: C25H41NO5Si2

SMILES: CCOC(=O)n1cc(CC(=O)O[Si](C)(C)C(C)(C)C)c2cc(O[Si](C)(C)C(C)(C)C)ccc21

Mol. weight [g/mol]: 491.77

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.89		Crippen Method
logp	7.121		Crippen Method
rinpol	2685.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R563834&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

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https://www.chemeo.com/cid/44-826-6/5-Hydroxyindoleacetic-acid-ethoxycarbonylated-TBDMS.pdf

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