3-Indolebutyric acid, ethoxycarbonylated, TBDMS

Inchi: InChI=1S/C21H31NO4Si/c1-7-25-20(24)22-15-16(17-12-8-9-13-18(17)22)11-10-14-19(23

InchiKey: ANZSAAHCKRNMEE-UHFFFAOYSA-N

Formula: C21H31NO4Si

SMILES: CCOC(=O)n1cc(CCCC(=O)O[Si](C)(C)C(C)(C)C)c2ccccc21

Mol. weight [g/mol]: 389.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.47		Crippen Method
logp	5.517		Crippen Method
rinpol	2419.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R563512&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices