

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(2)
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/ci9903071
Crippen Method:	https://www.cheméo.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

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