Indole, 3-(2-propionylaminoethyl), 5-methoxy, TMS

Inchi: InChI=1S/C17H26N2O2Si/c1-6-17(20)18-10-9-13-12-19(22(3,4)5)16-8-7-14(21-2)11-15(1

InchiKey: JVSSEWJSVPIWCG-UHFFFAOYSA-N

Formula: C17H26N2O2Si

SMILES: CCC(=O)NCCc1cn([Si](C)(C)C)c2ccc(OC)cc12

Mol. weight [g/mol]: 318.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.76		Crippen Method
logp	3.402		Crippen Method
rinpol	2425.00		NIST Webbook
rinpol	2425.00		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=R529067&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices