5-Methoxytryptophol, TMS

Inchi: InChI=1S/C17H29NO2Si2/c1-19-15-8-9-17-16(12-15)14(10-11-20-22(5,6)7)13-18(17)21(
InchiKey: ZZDMMBXZYBFWAP-UHFFFAOYSA-N
Formula: C17H29NO2Si2
SMILES: COc1ccc2c(c1)c(CCO[Si](C)(C)C)cn2[Si](C)(C)C
Mol. weight [g/mol]: 335.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.93		Crippen Method
logp	4.727		Crippen Method
rinpol	2092.00		NIST Webbook
rinpol	2088.00		NIST Webbook
rinpol	2088.00		NIST Webbook
rinpol	2092.00		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=R93882&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices