1-benzyl, 4,4,7,10-tetramethylsilatrane, c

Inchi: InChI=1S/C17H27NO3Si/c1-14-10-18-11-15(2)21-22(20-14,19-13-17(18,3)4)12-16-8-6-5

InchiKey: QKTHTNVMCPWGHL-UHFFFAOYSA-N

Formula: C17H27NO3Si

SMILES: CC1CN2CC(C)O[Si](Cc3ccccc3)(OCC2(C)C)O1

Mol. weight [g/mol]: 321.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.30		Crippen Method
logp	2.642		Crippen Method
rinpol	2138.00		NIST Webbook
rinpol	2138.00		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=R145530&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices