o-Vanilline, MO TMS

Inchi: InChI=1S/C12H19NO3Si/c1-14-12-10(9-13-15-2)7-6-8-11(12)16-17(3,4)5/h6-9H,1-5H3/b
InchiKey: JOYXHEXUVYKKCY-LCYFTJDESA-N
Formula: C12H19NO3Si
SMILES: CON=Cc1cccc(O[Si](C)(C)C)c1OC
Mol. weight [g/mol]: 253.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.75		Crippen Method
logp	2.889		Crippen Method
rinpol	1582.00		NIST Webbook
rinpol	1582.00		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=R92616&Units=SI

Legend

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