6-[12(Z)-Nonadecenyl]salicylic acid (2TMS)

Inchi: InChI=1S/C32H58O3Si2/c1-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-26-29-2
InchiKey: XKABAQWKVSFZDL-YPKPFQOOSA-N
Formula: C32H58O3Si2
SMILES: CCCCCCC=CCCCCCCCCCCCc1cccc(O[Si](C)(C)C)c1C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 546.97

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.38		Crippen Method
logp	10.862		Crippen Method
rinpol	3226.30		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U414067&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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