trans-2-Octenedioic acid, TMS

Inchi: InChI=1S/C14H28O4Si2/c1-19(2,3)17-13(15)11-9-7-8-10-12-14(16)18-20(4,5)6/h9,11H,7
InchiKey: QHCWAYVSWZJFGT-PKNBQFBNSA-N
Formula: C14H28O4Si2
SMILES: C[Si](C)(C)OC(=O)C=CCCCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 316.54

Physical Properties

Property code	Value	Unit	Source
log10ws	0.64		Crippen Method
logp	3.859		Crippen Method
rinpol	1738.00		NIST Webbook
rinpol	1738.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R583972&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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