6-Hydroxy-arachidic, methyl ester, tBDMS ether

Inchi: InChI=1S/C27H56O3Si/c1-8-9-10-11-12-13-14-15-16-17-18-19-22-25(23-20-21-24-26(28

InchiKey: JBJDUECARVBNET-UHFFFAOYSA-N

Formula: C27H56O3Si

SMILES: CCCCCCCCCCCCCCC(CCCCC(=O)OC)O[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]: 456.82

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.24		Crippen Method
logp	9.201		Crippen Method
rinpol	2739.00		NIST Webbook
rinpol	2739.00		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=R186848&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices