6-Hydroxy-stearic acid, methyl ester, tBDMS ether

Inchi: InChI=1S/C25H52O3Si/c1-8-9-10-11-12-13-14-15-16-17-20-23(21-18-19-22-24(26)27-5)28-29(6,7)25(2,3)4/h23H,8-22H2,1-7H3

InchiKey: LJCXJJZSIUCDRT-UHFFFAOYSA-N

Formula: C25H52O3Si

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

Mol. weight [g/mol]: 428.76

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.40		Crippen Method
logp	8.421		Crippen Method
rinpol	2542.00		NIST Webbook
rinpol	2542.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R186784&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