Palmitic acid, 2-tert-butyldimethylsilyloxy-, methyl ester

Other names: 2-Hydroxy-palmitic acid, methyl ester, 2-tBDMS ether
Methyl 2-hydroxyhexadecanoate, tbdms derivative

Inchi: InChI=1S/C23H48O3Si/c1-8-9-10-11-12-13-14-15-16-17-18-19-20-21(22(24)25-5)26-27(

InchiKey: JXIFMMAYTILMOV-UHFFFAOYSA-N

Formula: C23H48O3Si

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

Mol. weight [g/mol]: 400.71

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.56		Crippen Method
logp	7.641		Crippen Method
rinpol	2333.00		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=U314795&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices