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

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

InchiKey: VNMUQQRPWCUQHC-UHFFFAOYSA-N

Formula: C23H48O3Si

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

Mol. weight [g/mol]: 400.71

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.56		Crippen Method
logp	7.641		Crippen Method
rinpol	2341.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R186675&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

Latest version available from:

https://www.chemeo.com/cid/11-282-6/6-Hydroxy-palmitic-acid-methyl-ester-tBDMS-ether.pdf

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