

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

Inchi: InChI=1S/C25H52O3Si/c1-8-9-17-20-23(28-29(6,7)25(2,3)4)21-18-15-13-11-10-12-14-16
InchiKey: PDMQLEBNJNVTJP-UHFFFAOYSA-N
Formula: C25H52O3Si
SMILES: CCCCC(CCCCCCCCCC(=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	2575.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R187232&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Legend

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

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<https://www.chemeo.com/cid/54-188-4/13-Hydroxy-stearic-acid-methyl-ester-tBDMS-ether.pdf>

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