

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

Inchi: InChI=1S/C25H52O3Si/c1-8-9-20-23(28-29(6,7)25(2,3)4)21-18-16-14-12-10-11-13-15-17
InchiKey: NNRNJTFGDAPFOV-UHFFFAOYSA-N
Formula: C₂₅H₅₂O₃Si
SMILES: CCCCC(CCCCCCCCCCCCC(=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	2582.00		NIST Webbook
rinpol	2582.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R187183&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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.cheméo.com/cid/54-058-8/14-Hydroxy-stearic-acid-methyl-ester-tBDMS-ether.pdf>

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