Dodecanoic acid, 2-hydroxy, methyl ester, TMS

Inchi: InChI=1S/C16H34O3Si/c1-6-7-8-9-10-11-12-13-14-15(16(17)18-2)19-20(3,4)5/h15H,6-14

InchiKey: PHPBKGTVQKCOSS-UHFFFAOYSA-N

Formula: C16H34O3Si

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

Mol. weight [g/mol]: 302.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.63		Crippen Method
logp	4.910		Crippen Method
rinpol	1728.00		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=R383712&Units=SI

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/17-283-9/Dodecanoic-acid-2-hydroxy-methyl-ester-TMS.pdf

Generated by Cheméo on 2024-10-12 07:14:56.397478587 +0000 UTC m=+3298159.034447835.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.