

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

Inchi: InChI=1S/C24H50O3Si/c1-8-9-19-22(27-28(6,7)24(2,3)4)20-17-15-13-11-10-12-14-16-18
InchiKey: CBULPDBFELPIJR-UHFFFAOYSA-N
Formula: C24H50O3Si
SMILES: CCCCC(CCCCCCCCCC(=O)OC)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 414.74

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.98		Crippen Method
logp	8.031		Crippen Method
rinpol	2472.00		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=R187158&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/95-508-3/13-Hydroxy-heptadecanoic-acid-methyl-ester-tBDMS-ether.pdf>

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