

3-Hydroxy-heptadecanoic acid, methyl ester, 3-tBDMS ether

Inchi: InChI=1S/C24H50O3Si/c1-8-9-10-11-12-13-14-15-16-17-18-19-20-22(21-23(25)26-5)27-
InchiKey: OFIONSPXDHDDOA-UHFFFAOYSA-N
Formula: C₂₄H₅₀O₃Si
SMILES: CCCCCCCCCCCCCC(CC(=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	2447.00		NIST Webbook
rinpol	2447.00		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=R186853&Units=SI>

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/95-505-6/3-Hydroxy-heptadecanoic-acid-methyl-ester-3-tBDMS-ether.pdf>

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