

«alpha»-Hydroxyarachidic acid, TMSi-Me

Other names:	Eicosanoic acid, 2-hydroxy, methyl ester, TMS
Inchi:	InChI=1S/C24H50O3Si/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23(24(25)2
InchiKey:	AIDIPDFVXORXLT-UHFFFAOYSA-N
Formula:	C24H50O3Si
SMILES:	CCCCCCCCCCCCCCCCCCCC(O[Si](C)(C)C)C(=O)OC
Mol. weight [g/mol]:	414.74

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.98		Crippen Method
logp	8.031		Crippen Method
rinpol	2517.00		NIST Webbook
rinpol	2515.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R134213&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/37-282-8/alpha-Hydroxyarachidic-acid-TMSi-Me.pdf>

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