

ent-6«alpha»,7«alpha»,16«alpha»,17-(OH)4 KA, MeTMS

Inchi:	InChI=1S/C33H66O6Si4/c1-30-19-16-20-31(2,29(34)35-3)27(30)26(37-41(7,8)9)28(38-4
InchiKey:	FTYCAQJYLZNRFAF-AGSPEHARSA-N
Formula:	C33H66O6Si4
SMILES:	COC(=O)C1(C)CCCC2(C)C1C(O[Si](C)(C)C)C(O[Si](C)(C)C)C13CC(CCC21)C(CO[Si](C
Mol. weight [g/mol]:	671.22

Physical Properties

Property code	Value	Unit	Source
log10ws	0.48		Crippen Method
logp	8.674		Crippen Method
rmpol	2970.00		NIST Webbook
rmpol	2977.00		NIST Webbook
rmpol	2953.00		NIST Webbook
rmpol	2970.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R299340&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rmpol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/33-512-6/ent-6-alpha-7-alpha-16-alpha-17-OH-4-KA-MeTMS.pdf>

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