

ent-16«beta»,17-H2(OH)2

6«alpha»,7«alpha»(OH)2 kaurenoic acid,

MeTMSi

InchiKey:

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

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
rinpol	2988.00		NIST Webbook
rinpol	2989.00		NIST Webbook

Sources

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R258498&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

rinpol:

Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/66-915-3/ent-16-beta-17-H2-OH-2-6-alpha-7-alpha-OH-2-kaurenoic-acid-MeTMSi.pdf>

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