

16«alpha»,17-H2 (OH)2 GA34, MeTMS

Inchi: InChI=1S/C34H66O8Si4/c1-31-20-24(40-44(8,9)10)28(41-45(11,12)13)32(2,30(36)38-4)
InchiKey: FKRIIPRVKSLCOLF-UUKOHDQQSA-N
Formula: C34H66O8Si4
SMILES: COC(=O)C1C2C(C)(CC(O[Si](C)(C)C)C(O[Si](C)(C)C)C2(C)C(=O)OC)C2CCC3CC12CO
Mol. weight [g/mol]: 715.23

Physical Properties

Property code	Value	Unit	Source
log10ws	1.44		Crippen Method
logp	7.683		Crippen Method
rinpol	3033.00		NIST Webbook
rinpol	3036.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R299320&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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/24-478-5/16-alpha-17-H2-OH-2-GA34-MeTMS.pdf>

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