

GA17 (12-«alpha»-hydroxy), Me-TMS

Inchi: InChI=1S/C31H54O8Si3/c1-20-18-29-19-31(20,39-42(11,12)13)22(37-40(5,6)7)17-21(29)
InchiKey: QYJMNUMWIUSSEV-KXOCPAHSSA-N
Formula: C31H54O8Si3
SMILES: C=C1CC23CC1(O[Si](C)(C)C)C(O[Si](C)(C)C)CC2C1(C(=O)O[Si](C)(C)C)CCCC(C)(C(=O)O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 639.01

Physical Properties

Property code	Value	Unit	Source
log10ws	0.08		Crippen Method
logp	6.300		Crippen Method
rinpol	2631.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R539074&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/38-008-1/GA17-12-alpha-hydroxy-Me-TMS.pdf>

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