

2«beta»-OH-GA84 methyl ester TMS ether

Inchi: InChI=1S/C29H50O7Si3/c1-18-15-27-17-28(18,36-39(10,11)12)16-19(34-37(4,5)6)22(27)
InchiKey: FKLYZWSCTUZMCU-ISQJTZJUSA-N
Formula: C29H50O7Si3
SMILES: C=C1CC23CC1(O[Si](C)(C)C)CC(O[Si](C)(C)C)C2C12CCC(O[Si](C)(C)C)C(C)(C(=O)O)
Mol. weight [g/mol]: 594.96

Physical Properties

Property code	Value	Unit	Source
log10ws	0.33		Crippen Method
logp	5.888		Crippen Method
rinpol	2655.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R181343&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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