

16,17-Dihydro-17-OH-GA53 methyl ester TMS ether

Other names: GA53, 16,17-dihydro-17-ol, methyl ester TMS ether
Inchi: InChI=1S/C28H50O6Si2/c1-25-13-11-14-26(2,24(30)32-4)22(25)21(23(29)31-3)27-16-19
InchiKey: IBWSUNLYMOKQBR-KZQTXCAMSA-N
Formula: C28H50O6Si2
SMILES: COC(=O)C1C2C(C)(C(=O)OC)CCCC2(C)C2CCC3(O[Si](C)(C)C)CC12CC3CO[Si](C)(C)
Mol. weight [g/mol]: 538.86

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.54		Crippen Method
logp	6.023		Crippen Method
rinpol	2750.00		NIST Webbook
rinpol	2774.00		NIST Webbook
rinpol	2776.00		NIST Webbook
rinpol	2774.00		NIST Webbook
rinpol	2750.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R169729&Units=SI>

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/65-989-3/16-17-Dihydro-17-OH-GA53-methyl-ester-TMS-ether.pdf>

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