

17-OH-GA53 methyl ester TMS ether

Other names: 17-OH-GA53, MeTMS
Inchi: InChI=1S/C28H48O6Si2/c1-25-13-11-14-26(2,24(30)32-4)22(25)21(23(29)31-3)27-16-19
InchiKey: ULHRGZPJCAVDNX-KEQUQHISSA-N
Formula: C₂₈H₄₈O₆Si₂
SMILES: COC(=O)C1C2C(C)(C(=O)OC)CCCC2(C)C2CCC3(O[Si](C)(C)C)CC12CC3=CO[Si](C)(C)C
Mol. weight [g/mol]: 536.85

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.13		Crippen Method
logp	6.291		Crippen Method
rinpol	2708.00		NIST Webbook
rinpol	2708.00		NIST Webbook
rinpol	2709.00		NIST Webbook
rinpol	2707.00		NIST Webbook
rinpol	2707.00		NIST Webbook
rinpol	2707.00		NIST Webbook
rinpol	2708.00		NIST Webbook
rinpol	2709.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R174939&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

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