

2«beta»-OH GA53 methyl ester TMS ether

Other names: GA97 methyl ester TMS ether
Inchi: InChI=1S/C28H48O6Si2/c1-18-14-27-17-28(18,34-36(9,10)11)13-12-20(27)25(2)15-19(3
InchiKey: KSRYZLCYMIFGNF-ZHUQCEIBSA-N
Formula: C28H48O6Si2
SMILES: C=C1CC23CC1(O[Si](C)(C)C)CCC2C1(C)CC(O[Si](C)(C)C)CC(C)(C(=O)OC)C1C3C(=O
Mol. weight [g/mol]: 536.85

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.75		Crippen Method
logp	5.942		Crippen Method
rinpola	2695.00		NIST Webbook
rinpola	2675.00		NIST Webbook
rinpola	2701.00		NIST Webbook
rinpola	2702.00		NIST Webbook
rinpola	2680.00		NIST Webbook
rinpola	2651.00		NIST Webbook
rinpola	2680.00		NIST Webbook
rinpola	2680.00		NIST Webbook
rinpola	2658.00		NIST Webbook
rinpola	2674.00		NIST Webbook
rinpola	2699.00		NIST Webbook
rinpola	2690.00		NIST Webbook
rinpola	2695.00		NIST Webbook
rinpola	2692.00		NIST Webbook
rinpola	2695.00		NIST Webbook
rinpola	2699.00		NIST Webbook
rinpola	2658.00		NIST Webbook
rinpola	2701.00		NIST Webbook
rinpola	2680.00		NIST Webbook
rinpola	2695.00		NIST Webbook
rinpola	2674.00		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=R169709&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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