

GA74, MeTMS

Other names: GA74, methyl ester TMS
GA74 methyl ester TMS ether
12-«alpha»-Hydroxy-GA14, methyl ester, TMS

Inchi: InChI=1S/C28H48O6Si2/c1-17-15-28-16-18(17)19(33-35(6,7)8)14-20(28)26(2)13-12-21(3)

InchiKey: RUQHTXLJSAGIIL-CBZWRZRMSA-N

Formula: C28H48O6Si2

SMILES: C=C1CC23CC1C(O[Si](C)(C)C)CC2C1(C)CCC(O[Si](C)(C)C)C(C)(C(=O)OC)C1C3C(=O)C

Mol. weight [g/mol]: 536.85

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.51		Crippen Method
logp	5.797		Crippen Method
rinpol	2682.00		NIST Webbook
rinpol	2683.00		NIST Webbook
rinpol	2693.00		NIST Webbook
rinpol	2700.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R79903&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/49-339-2/GA74-MeTMS.pdf>

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