

12-OH GA14 methyl ester TMS ether

Inchi: InChI=1S/C25H40O5Si/c1-15-13-25-14-16(15)9-10-17(25)23(2)12-11-18(30-31(6,7)8)24
InchiKey: QQEYOHKHRLMQMP-XPBYACCWSA-N
Formula: C₂₅H₄₀O₅Si
SMILES: C=C1CC23CC1CCC2C1(C)CCC(O[Si](C)(C)C)C(C)(C(=O)OC)C1C3C(=O)OC
Mol. weight [g/mol]: 448.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.00		Crippen Method
logp	4.967		Crippen Method
rinpol	2709.00		NIST Webbook
rinpol	2689.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R204456&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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/26-305-4/12-OH-GA14-methyl-ester-TMS-ether.pdf>

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