

18-OH-GA4 methyl ester TMS ether

Inchi: InChI=1S/C25H40O6Si2/c1-15-13-23-14-16(15)9-10-17(23)24-12-11-18(30-32(3,4)5)25(30-32(3,4)5)25(30-32(3,4)5)
InchiKey: ZEXCDJJGTUYFMR-RCNSMDSDSA-N
Formula: C25H40O6Si2
SMILES: C=C1CC23CC1CCC2C12CCC(O[Si](C)(C)C)C(O[Si](C)(C)C)(C(=O)O1)C2C3C(=O)OC3C1
Mol. weight [g/mol]: 492.75

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.74		Crippen Method
logp	4.668		Crippen Method
rinpol	2634.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R151827&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/83-867-8/18-OH-GA4-methyl-ester-TMS-ether.pdf>

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