

# 12«beta»-OH-GA4 methyl ester TMS ether

<b>Other names:</b>	[13C] GA71 methyl ester TMS ether
<b>Inchi:</b>	InChI=1S/C26H42O6Si2/c1-15-13-25-14-16(15)17(31-33(4,5)6)12-18(25)26-11-10-19(32)
<b>InchiKey:</b>	YJIAMACEKPLATL-MJQUMQIQSA-N
<b>Formula:</b>	C26H42O6Si2
<b>SMILES:</b>	C=C1CC23CC1C(O[Si](C)(C)C)CC2C12CCC(O[Si](C)(C)C)C(C)(C(=O)O1)C2C3C(=O)C
<b>Mol. weight [g/mol]:</b>	506.78

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.92		Crippen Method
logp	4.914		Crippen Method
rinpola	2695.00		NIST Webbook
rinpola	2683.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R151758&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R151758&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>rinpola:</b>	Non-polar retention indices

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<https://www.chemeo.com/cid/34-605-2/12-beta-OH-GA4-methyl-ester-TMS-ether.pdf>

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