

# [13C]16-epi-GA82 methyl ester TMS ether

<b>Other names:</b>	16-epi-GA82 methyl ester TMS ether
<b>Inchi:</b>	InChI=1S/C26H44O6Si2/c1-24-19(32-34(6,7)8)11-12-26(31-23(24)28)18-10-9-16-13-25(
<b>InchiKey:</b>	VQPGMENVKJBWHH-YHMOOJIJSA-N
<b>Formula:</b>	C26H44O6Si2
<b>SMILES:</b>	COC(=O)C1C2C3(CCC(O[Si](C)(C)C)C2(C)C(=O)O3)C2CCC3CC12CC3CO[Si](C)(C)C
<b>Mol. weight [g/mol]:</b>	508.80

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.71		Crippen Method
logp	4.995		Crippen Method
rinpola	2822.00		NIST Webbook
rinpola	2821.00		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=R176826&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R176826&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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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