

# GA31, MeTMS

<b>Other names:</b>	GA31 methyl ester TMS ether
<b>Inchi:</b>	InChI=1S/C23H32O5Si/c1-13-11-22-12-14(13)15(28-29(4,5)6)10-16(22)23-9-7-8-21(2,20)
<b>InchiKey:</b>	YTEJWGMOWVRFPFPM-FNXSURMMSA-N
<b>Formula:</b>	C <sub>23</sub> H <sub>32</sub> O <sub>5</sub> Si
<b>SMILES:</b>	<chem>C=C1CC23CC1C(O[Si](C)(C)C)CC2C12CC=CC(C)(C(=O)O1)C2C3C(=O)OC</chem>
<b>Mol. weight [g/mol]:</b>	416.58

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.27		Crippen Method
logp	3.860		Crippen Method
rinpola	2550.00		NIST Webbook
rinpola	2564.00		NIST Webbook
rinpola	2550.00		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=R79430&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R79430&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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<https://www.chemeo.com/cid/52-082-3/GA31-MeTMS.pdf>

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