

# iso[14C] GA3 methyl ester TMS ether

**Other names:** isoGA3 methyl ester TMS ether  
**Inchi:** InChI=1S/C26H40O6Si2/c1-16-14-24-15-25(16,32-34(7,8)9)12-10-17(24)26-13-11-18(31)  
**InchiKey:** QJSHIGDRCGMRDL-YGAWNTLJSA-N  
**Formula:** C<sub>26</sub>H<sub>40</sub>O<sub>6</sub>Si<sub>2</sub>  
**SMILES:** C=C1CC23CC1(O[Si](C)(C)C)CCC2C12C=CC(O[Si](C)(C)C)C(C)(C(=O)O1)C2C3C(=O)  
**Mol. weight [g/mol]:** 504.76

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.02		Crippen Method
logp	4.834		Crippen Method
rinpol	2633.00		NIST Webbook
rinpol	2625.00		NIST Webbook
rinpol	2645.00		NIST Webbook
rinpol	2645.00		NIST Webbook
rinpol	2633.00		NIST Webbook
rinpol	2645.00		NIST Webbook
rinpol	2633.00		NIST Webbook
rinpol	2640.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R191023&Units=SI>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**rinpol:** Non-polar retention indices

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