

[14C] GA7 di-acid 9,10-ene, methyl ester TMS ether

Inchi:	InChI=1S/C26H40O5Si2/c1-16-14-26-15-17(16)10-12-19(26)18-11-13-20(30-32(4,5)6)25
InchiKey:	PHPDUMKOJSFWJK-ZPKFEUISSA-N
Formula:	C26H40O5Si2
SMILES:	C=C1CC23CC1CCC2=C1C=CC(O[Si](C)(C)C)C(C)(C(=O)O[Si](C)(C)C)C1C3C(=O)OC
Mol. weight [g/mol]:	488.76

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.66		Crippen Method
logp	5.623		Crippen Method
rinpol	2399.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R190931&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/13-376-0/14C-GA7-di-acid-9-10-ene-methyl-ester-TMS-ether.pdf>

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