[14C1]GA7 methyl ester TMS ether

Other names:	GA7 methyl ester TMS ether
Inchi:	InChI=1S/C23H32O5Si/c1-13-11-22-12-14(13)7-8-15(22)23-10-9-16(28-29(4,5)6)21(2,20
InchiKey:	QYWOOSKTNLXOPW-DTOPKNIOSA-N
Formula:	C23H32O5Si
SMILES:	C=C1CC23CC1CCC2C12C=CC(O[Si](C)(C)C)C(C)(C(=O)O1)C2C3C(=O)OC
Mol. weight [g/mol]:	416.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.27		Crippen Method
logp	3.860		Crippen Method
rinpol	2520.00		NIST Webbook
rinpol	2525.00		NIST Webbook
rinpol	2520.00		NIST Webbook
rinpol	2522.00		NIST Webbook
rinpol	2525.00		NIST Webbook
rinpol	2521.00		NIST Webbook
rinpol	2521.00		NIST Webbook
rinpol	2522.00		NIST Webbook
rinpol	2522.00		NIST Webbook
rinpol	2519.00		NIST Webbook
rinpol	2511.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R183854&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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/29-733-6/14C1-GA7-methyl-ester-TMS-ether.pdf