[14C1]GA44 methyl ester

Inchi:	InChI=1S/C24H36O5Si/c1-15-12-23-13-24(15,29-30(4,5)6)11-8-16(23)22-10-7-9-21(2,20
InchiKey:	DOKNGJSNWBXFCM-RMSVLQMSSA-N
Formula:	C24H36O5Si
SMILES:	C=C1CC23CC1(O[Si](C)(C)C)CCC2C12CCCC(C)(C(=O)OC1)C2C3C(=O)OC
Mol. weight [g/mol]:	432.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.72		Crippen Method
logp	4.476		Crippen Method
rinpol	2778.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R392924&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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/55-319-7/14C1-GA44-methyl-ester.pdf

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