

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

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