

[13C]endo-GA4 methyl ester TMS ether

Other names: [14C1]GA4 methyl ester TMS ether
Inchi: InChI=1S/C23H34O5Si/c1-13-11-22-12-14(13)7-8-15(22)23-10-9-16(28-29(4,5)6)21(2,20)
InchiKey: ATWIBZVZMYFKOI-DTOPKNIOSA-N
Formula: C23H34O5Si
SMILES: C=C1CC23CC1CCC2C12CCC(O[Si](C)(C)C)C(C)(C(=O)O1)C2C3C(=O)OC
Mol. weight [g/mol]: 418.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.41		Crippen Method
logp	4.084		Crippen Method
rinpol	2517.00		NIST Webbook
rinpol	2511.00		NIST Webbook
rinpol	2481.00		NIST Webbook
rinpol	2478.00		NIST Webbook
rinpol	2515.00		NIST Webbook
rinpol	2498.00		NIST Webbook
rinpol	2517.00		NIST Webbook
rinpol	2517.00		NIST Webbook
rinpol	2517.00		NIST Webbook
rinpol	2518.00		NIST Webbook
rinpol	2498.00		NIST Webbook
rinpol	2521.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R176851&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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