

[13C]endo-GA1 methyl ester TMS ether

Inchi: InChI=1S/C26H42O6Si2/c1-16-14-24-15-25(16,32-34(7,8)9)12-10-17(24)26-13-11-18(31)
InchiKey: UOYZRHLGPUDVGI-GJUFPDMZSA-N
Formula: C26H42O6Si2
SMILES: C=C1CC23CC1(O[Si](C)(C)C)CCC2C1CCC(O[Si](C)(C)C)C(C)(C(=O)O1)C2C3C(=O)C
Mol. weight [g/mol]: 506.78

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.16		Crippen Method
logp	5.058		Crippen Method
rinpol	2676.00		NIST Webbook
rinpol	2647.00		NIST Webbook
rinpol	2724.00		NIST Webbook
rinpol	2635.00		NIST Webbook
rinpol	2635.00		NIST Webbook
rinpol	2670.00		NIST Webbook
rinpol	2670.00		NIST Webbook
rinpol	2670.00		NIST Webbook
rinpol	2674.00		NIST Webbook
rinpol	2674.00		NIST Webbook
rinpol	2674.00		NIST Webbook
rinpol	2671.00		NIST Webbook
rinpol	2676.00		NIST Webbook
rinpol	2676.00		NIST Webbook
rinpol	2667.00		NIST Webbook
rinpol	2668.00		NIST Webbook
rinpol	2677.00		NIST Webbook
rinpol	2678.00		NIST Webbook
rinpol	2681.00		NIST Webbook
rinpol	2682.00		NIST Webbook
rinpol	2635.00		NIST Webbook
rinpol	2670.00		NIST Webbook
rinpol	2674.00		NIST Webbook
rinpol	2668.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R178708&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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