

[13C]3-epi-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-LZXYUWHESA-N
Formula: C26H42O6Si2
SMILES: C=C1CC23CC1(O[Si](C)(C)C)CCC2C12CCC(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	2795.00		NIST Webbook
rinpol	2793.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R319954&Units=SI>

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/53-421-5/13C-3-epi-GA1-methyl-ester-TMS-ether.pdf>

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