

[13C]GA3 methyl ester TMS ether

Other names: [14C] GA3 methyl ester TMS ether
Inchi: InChI=1S/C26H40O6Si2/c1-16-14-24-15-25(16,32-34(7,8)9)12-10-17(24)26-13-11-18(31)
InchiKey: QJSHIGDRCGMRDL-GJUFPMZSA-N
Formula: C26H40O6Si2
SMILES: C=C1CC23CC1(O[Si](C)(C)C)CCC2C12C=CC(O[Si](C)(C)C)C(C)(C(=O)O1)C2C3C(=O)
Mol. weight [g/mol]: 504.76

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.02		Crippen Method
logp	4.834		Crippen Method
rinpol	2685.00		NIST Webbook
rinpol	2687.00		NIST Webbook
rinpol	2697.00		NIST Webbook
rinpol	2691.00		NIST Webbook
rinpol	2703.00		NIST Webbook
rinpol	2705.00		NIST Webbook
rinpol	2709.00		NIST Webbook
rinpol	2712.00		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=R181576&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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