

[13C]15-epi-GA63 methyl ester TMS ether

Inchi: InChI=1S/C26H42O6Si2/c1-15-16-10-11-17-25(14-16,21(15)32-34(7,8)9)19(22(27)29-3)
InchiKey: JHMFVYHNXOBDPJ-AURSPKMCSA-N
Formula: C26H42O6Si2
SMILES: C=C1C2CCC3C45CCC(O[Si](C)(C)C(C)(C(=O)O4)C5C(C(=O)OC)C3(C2)C1O[Si](C)(C)C
Mol. weight [g/mol]: 506.78

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -0.92 | | Crippen Method |
| logp | 4.914 | | Crippen Method |
| rinpol | 2786.00 | | NIST Webbook |

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R176806&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/34-200-1/13C-15-epi-GA63-methyl-ester-TMS-ether.pdf>

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