

2-«alpha»-Hydroxy-9,15-cyclo-GA9, methyl ester [D2], TMS

Inchi: InChI=1S/C23H32O5Si/c1-12-13-7-8-22-16(12)21(22,9-13)15(18(24)26-3)17-20(2)10-14
InchiKey: JLZFFKANKJYMMT-SKLKLVQMSA-N
Formula: C₂₃H₃₂O₅Si
SMILES: C=C1C2CCC34C1C3(C2)C(C(=O)OC)C1C2(C)CC(O[Si](C)(C)C)CC14OC2=O
Mol. weight [g/mol]: 416.58

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -2.07 | | Crippen Method |
| logp | 3.694 | | Crippen Method |
| rinpol | 2466.00 | | NIST Webbook |
| rinpol | 2471.00 | | NIST Webbook |

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R499793&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/27-544-8/2-alpha-Hydroxy-9-15-cyclo-GA9-methyl-ester-D2-TMS.pdf>

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