

2«beta»-hydroxy-9,15-cyclo-GA9 (GA105), MeTMS

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| 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-XIYYVQIMSA-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 | 2441.00 | | NIST Webbook |
| rinpol | 2443.00 | | NIST Webbook |
| rinpol | 2441.00 | | NIST Webbook |

Sources

| | |
|-----------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R224247&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

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/55-110-8/2-beta-hydroxy-9-15-cyclo-GA9-GA105-MeTMS.pdf>

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