

3A,11B,17A,21-Tetrahydroxy-5B-pregnan-20-one, MO TMS

Other names: 5«beta»-Pregnane-3«alpha», 11«beta», 17«alpha», 21-tetrol-20-one (THF), MO TMS
Inchi: InChI=1S/C34H69NO5Si4/c1-32-20-18-26(38-42(7,8)9)22-25(32)16-17-27-28-19-21-34(4)5
InchiKey: WZZDCZPDFSSOIG-IKUUVTFOSA-N
Formula: C34H69NO5Si4
SMILES: CON=C(CO[Si](C)(C)C)C1(O[Si](C)(C)C)CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3C
Mol. weight [g/mol]: 684.26

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -0.31 | | Crippen Method |
| logp | 9.523 | | Crippen Method |
| rinpol | 3032.00 | | NIST Webbook |
| rinpol | 3038.00 | | NIST Webbook |
| rinpol | 3023.00 | | NIST Webbook |
| rinpol | 3039.00 | | NIST Webbook |
| rinpol | 3038.00 | | NIST Webbook |
| rinpol | 3027.00 | | NIST Webbook |
| rinpol | 3041.00 | | 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=R486029&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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