

5-Pregnen-3«beta»,20«alpha»-diol, TBDMS

Inchi: InChI=1S/C33H62O2Si2/c1-23(34-36(10,11)30(2,3)4)27-16-17-28-26-15-14-24-22-25(35)
InchiKey: BUSSZAFGSKFLCU-PLWCNECCSA-N
Formula: C33H62O2Si2
SMILES: CC(O[Si](C)(C)C(C)(C)C)C1CCC2C3CC=C4CC(O[Si](C)(C)C(C)(C)C)CCC4(C)C3CCC1
Mol. weight [g/mol]: 547.02

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -6.12 | | Crippen Method |
| logp | 10.366 | | Crippen Method |
| rinpol | 3417.00 | | NIST Webbook |
| rinpol | 3417.00 | | 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=R526266&Units=SI>

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/68-674-9/5-Pregnen-3-beta-20-alpha-diol-TBDMS.pdf>

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