

5-Pregnen-3«beta»,17«alpha»,20«alpha»-triol, (VDMS)3

Inchi: InChI=1S/C33H58O3Si3/c1-13-37(7,8)34-25(4)33(36-39(11,12)15-3)23-20-30-28-17-16-7
InchiKey: YCLSEJHWTWQAIT-RXBRCWFPSA-N
Formula: C33H58O3Si3
SMILES: C=C[Si](C)(C)OC1CCC2(C)C(=CCC3C2CCC2(C)C3CCC2(O[Si](C)(C)C=C)C(C)O[Si](C)(C)C=C)C(C)O[Si](C)(C)C=C
Mol. weight [g/mol]: 587.07

Physical Properties

| Property code | Value | Unit | Source |
|---------------|-------|------|----------------|
| log10ws | -3.43 | | Crippen Method |
| logp | 9.286 | | Crippen Method |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R529547&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

Latest version available from:

<https://www.chemeo.com/cid/97-222-8/5-Pregnen-3-beta-17-alpha-20-alpha-triol-VDMS-3.pdf>

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