

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

Inchi: InChI=1S/C32H62O2Si2/c1-22(33-35(9,10)30(2,3)4)28-17-18-29-27-15-13-23-21-24(34-36)25-26
InchiKey: CTISISFGSJXHDD-HHRFASEAUSA-N
Formula: C32H62O2Si2
SMILES: CC(O[Si](C)(C)C(C)(C)C)C1CCC2C3CCC4CC(O[Si](C)(C)C(C)(C)C)CCC4C3CCC12C
Mol. weight [g/mol]: 535.00

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.60		Crippen Method
logp	10.056		Crippen Method
rinpol	3231.00		NIST Webbook
rinpol	3231.00		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=R526226&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/62-502-5/5-beta-Pregnan-3-alpha-20-beta-diol-TBDMS.pdf>

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