

5«beta»-Pregnane-3«alpha»,17«alpha»,20«alpha»-triol-3-20-O-diTBDMSi

InChI: C33H64O3Si2/c1-23(35-37(10,11)29(2,3)4)33(34)21-18-28-26-15-14-24-22-25
InChIKey: GHNXJGWJFKLUHM-ZNWXLFBDNA-N
Formula: C₃₃H₆₄O₃Si₂
SMILES: CC(O[Si](C)(C)C(C)(C)C)C1(O)CCC2C3CCC4CC(O[Si](C)(C)C(C)(C)C)CCC4(C)C3CCO
Mol. weight [g/mol]: 565.03

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.64		Crippen Method
logp	9.561		Crippen Method
rinpol	3460.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R144240&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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<https://www.chemeo.com/cid/10-421-2/5-beta-Pregnane-3-alpha-17-alpha-20-alpha-triol-3-20-O-diTBDMSi.pdf>

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