

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

InChI: InChI=1S/C36H66O3Si2/c1-26(2)40(21-9-10-22-40)39-29-15-18-34(7)28(25-29)13-14-30(3,20-O)-diTMTBSi
InChIKey: UHNPDTLWGFMEK-CZOFRFMYSA-N
Formula: C36H66O3Si2
SMILES: CC(O[Si]1(C(C)(C)C)CCCC1)C1(O)CCC2C3CCC4CC(O[Si]5(C(C)C)CCCC5)CCC4(C)C
Mol. weight [g/mol]: 603.08

Physical Properties

Property code	Value	Unit	Source
logp	10.239		Crippen Method
rinpol	4109.00		NIST Webbook
rinpol	4109.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R144275&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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