

17«alpha»,20«beta»,21-Trihydroxypregn-4-en-3-one

bis-TMS

InChI=1S/C27H48O4Si2/c1-25-14-11-20(28)17-19(25)9-10-21-22(25)12-15-26(2)23(21)1

InChIKey: XLLYCXNDPZWFEF-XOFIXHOESA-N

Formula: C27H48O4Si2

SMILES: CC12CCC(=O)C=C1CCC1C2CCC2(C)C1CCC2(O)C(CO[Si](C)(C)C)O[Si](C)(C)C

Mol. weight [g/mol]: 492.84

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.39		Crippen Method
logp	6.321		Crippen Method
rinpol	3220.00		NIST Webbook
rinpol	3220.00		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=R525005&Units=SI>

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/56-004-5/17-alpha-20-beta-21-Trihydroxypregn-4-en-3-one-bis-TMS.pdf>

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