

17-«beta»-Hydroxy-7-«alpha»,17-«alpha»-dimethyl-5-beta-androstan-3-one-per-TMS

InChI: InChI=1S/C27H50O2Si2/c1-19-17-20-18-21(28-30(5,6)7)11-14-25(20,2)22-12-15-26(3)27-31
InChIKey: ZDOMRCSGCGJJBFH-SEIWIAKHSA-N
Formula: C27H50O2Si2
SMILES: CC1CC2C=C(O[Si](C)(C)C)CCC2(C)C2CCC3(C)C(CCC3(C)O[Si](C)(C)C)C12
Mol. weight [g/mol]: 462.86

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.75		Crippen Method
logp	8.231		Crippen Method
rinpol	2683.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R257435&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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