

5«beta»-Androstan-3«beta»-ol-17-one, TBDMS

Inchi: InChI=1S/C31H58O2Si2/c1-28(2,3)34(9,10)32-23-17-19-30(7)22(21-23)13-14-24-25-15-
InchiKey: CLHFTFZHPTFECO-JCDRPODTSA-N
Formula: C31H58O2Si2
SMILES: CC12CCC3C(CCC4CC(O[Si](C)(C)C(C)(C)C)CCC43C)C1CC=C2O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 518.96

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.66		Crippen Method
logp	9.935		Crippen Method
rinpol	2693.00		NIST Webbook
rinpol	2693.00		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=R526206&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/52-498-2/5-beta-Androstan-3-beta-ol-17-one-TBDMS.pdf>

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