

3B,16A-Dihydroxy-5-androsten-17-one, MO TMS

Inchi: InChI=1S/C26H49NO3Si2/c1-25-14-12-19(29-31(4,5)6)16-18(25)10-11-20-21(25)13-15-2
InchiKey: TVJNIUFLVUUMNG-VGPBRKECSA-N
Formula: C26H49NO3Si2
SMILES: CON=C1C(O[Si](C)(C)C)CC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 479.84

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.58		Crippen Method
logp	7.082		Crippen Method
rinpol	2732.00		NIST Webbook
rinpol	2768.00		NIST Webbook
rinpol	2774.00		NIST Webbook
rinpol	2743.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R486034&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/46-065-9/3B-16A-Dihydroxy-5-androsten-17-one-MO-TMS.pdf>

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