

3-«beta»,19-Dihydroxy-5-androsten-17-one, MO TMS

Inchi: InChI=1S/C26H47NO3Si2/c1-25-15-13-20(30-32(6,7)8)17-19(25)9-10-21-22(25)14-16-26
InchiKey: TXXVJPSOKAEKFI-NNYBWSOPSA-N
Formula: C26H47NO3Si2
SMILES: CON=C1CCC2C3CC=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC12CO[Si](C)(C)C
Mol. weight [g/mol]: 477.83

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.56		Crippen Method
logp	7.003		Crippen Method
rinpol	2705.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R386033&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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