17«alpha»-hydroxy-5«alpha»-androstan-3-one (3-enol), per-TMS

Inchi: InChI=1S/C25H46O2Si2/c1-24-15-13-19(26-28(3,4)5)17-18(24)9-10-20-21-11-12-23(27-

InchiKey: SJQAAFBSGVNPLH-STHJLMPXSA-N

Formula: C25H46O2Si2

SMILES: CC12CCC(O[Si](C)(C)C)=CC1CCC1C2CCC2(C)C(O[Si](C)(C)C)CCC12

Mol. weight [g/mol]: 434.80

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.15		Crippen Method
logp	7.594		Crippen Method
rinpol	2563.00		NIST Webbook
rinpol	2636.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R518344&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices