5-«alpha»-Androstan-7-«alpha»,17-«beta»-diol, TMS

Inchi: InChI=1S/C25H48O2Si2/c1-24-15-10-9-11-18(24)17-21(26-28(3,4)5)23-19-12-13-22(27-
InchiKey: MJMIFJGLEHUVMI-XTDPNHJSSA-N
Formula: C25H48O2Si2
SMILES: CC12CCCCC1CC(O[Si](C)(C)C)C1C2CCC2(C)C(O[Si](C)(C)C)CCC12
Mol. weight [g/mol]: 436.82

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.92		Crippen Method
logp	7.469		Crippen Method
rinpol	2437.00		NIST Webbook
rinpol	2430.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R384908&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