5-«beta»-Androstan-3-«beta»,17-«alpha»-diol, TMS

Other names: 5«beta»-Androstanediol-3«beta»,17«alpha», bis-TMS
Inchi: InChI=1S/C25H48O2Si2/c1-24-15-13-19(26-28(3,4)5)17-18(24)9-10-20-21-11-12-23(27-
InchiKey: KBSHKNYEUGMMDQ-NBFLWYEDSA-N
Formula: C25H48O2Si2
SMILES: CC12CCC(O[Si](C)(C)C)CC1CCC1C2CCC2(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	2474.00		NIST Webbook
rinpol	2469.00		NIST Webbook
rinpol	2486.00		NIST Webbook
rinpol	2460.00		NIST Webbook
rinpol	2469.00		NIST Webbook
rinpol	2460.00		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=R297740&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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