Androstan-17-one, 3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-, (3«alpha»,5«beta»)-

Other names: Etiocholan-3«alpha»-ol-17-one, tert-butyldimethylsilyl ether
3-«alpha»-tert-butyldimethylsilyloxy-5-«beta»-androstan-17-one
Ethiocholan-3«alpha»-ol-17-one, tert-butyldimethylsilyl ether

Inchi: InChI=1S/C25H44O2Si/c1-23(2,3)28(6,7)27-18-12-14-24(4)17(16-18)8-9-19-20-10-11-22

InchiKey: UGWVQACEZWDYMD-KZENVJRNSA-N

Formula: C25H44O2Si

SMILES: CC12CCC3C(CCC4CC(O[Si](C)(C)C(C)(C)C)CCC43C)C1CCC2=O

Mol. weight [g/mol]: 404.70

CAS: 65598-73-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.95		Crippen Method
logp	6.989		Crippen Method
rinpol	2810.40		NIST Webbook
rinpol	2814.30		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C65598734&Units=SI

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

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices