trans-Androsterone, tert-butyldimethylsilyl ether

Other names: Androsterone, (e)-, tbdms derivative
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-UHFFFAOYSA-N
Formula: C25H44O2Si
SMILES: CC12CCC3C(CCC4CC(O[Si](C)(C)C(C)(C)C)CCC43C)C1CCC2=O
Mol. weight [g/mol]: 404.70

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.95		Crippen Method
logp	6.989		Crippen Method
rinpol	2904.50		NIST Webbook
rinpol	2904.50		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=C65598734&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices