5«alpha»-Androstan-3,17-dione, 3,17-bis(trimethylsilyl) enol ether

Other names: 5A-Androstanedione (5A-Androstan-3,17-dione), TMS

Inchi: InChI=1S/C25H44O2Si2/c1-24-15-13-19(26-28(3,4)5)17-18(24)9-10-20-21-11-12-23(27-

InchiKey: RJIVKCCIVQDMHQ-UHFFFAOYSA-N

Formula: C25H44O2Si2

SMILES: CC12CCC3C(CCC4CC(O[Si](C)(C)C)=CCC43C)C1CC=C2O[Si](C)(C)C

Mol. weight [g/mol]: 432.79

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.39		Crippen Method
logp	7.720		Crippen Method
rinpol	2645.00		NIST Webbook
rinpol	2645.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U308778&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