Androst-5-en-17-one, 3-[(trimethylsilyl)oxy]-, (3«beta»)-

Other names: Androst-5-en-17-one, 3«beta»-(trimethylsiloxy)-
Androst-5-en-3«beta»-ol-17-one, TMS
Dehydroepiandrosterone, TMS
Dehydroepiandrosterone, TMSi (3-O)
Androsterone, mono-TMS
Dehydroepiandrosterone, (3«beta»)-, tms derivative

Inchi: InChI=1S/C22H36O2Si/c1-21-12-10-16(24-25(3,4)5)14-15(21)6-7-17-18-8-9-20(23)22(18

InchiKey: BVHPVDOXVFBYNL-OWXTWKKPSA-N

Formula: C22H36O2Si

SMILES: CC12CCC3C(CC=C4CC(O[Si](C)(C)C)CCC43C)C1CCC2=O

Mol. weight [g/mol]: 360.61

CAS: 3747-91-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.79		Crippen Method
logp	5.738		Crippen Method
rinpol	2555.00		NIST Webbook
rinpol	2524.00		NIST Webbook
rinpol	2574.00		NIST Webbook
rinpol	2568.00		NIST Webbook
rinpol	2584.00		NIST Webbook
rinpol	2568.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3747919&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