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

Other names: 5«beta»-Androstan-17-one, 3«alpha»-(trimethylsiloxy)-
3«alpha»-Trimethylsilyloxy-5«beta»-androstan-17-one
5«beta»-Androstan-3«alpha»-ol-17-one, TMS
Etiocholanolone, mono-TMS
Etiocholanolone TMS
Etiocholanone, tms derivative

Inchi: InChI=1S/C22H38O2Si/c1-21-12-10-16(24-25(3,4)5)14-15(21)6-7-17-18-8-9-20(23)22(18

InchiKey: RKALSSDGCWGKHQ-BLXKWZJGSA-N

Formula: C22H38O2Si

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

Mol. weight [g/mol]: 362.62

CAS: 4867-14-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.69		Crippen Method
logp	5.818		Crippen Method
rinpol	2521.00		NIST Webbook
rinpol	2527.00		NIST Webbook
rinpol	2548.00		NIST Webbook
rinpol	2556.00		NIST Webbook
rinpol	2521.00		NIST Webbook
rinpol	2575.80		NIST Webbook
rinpol	2513.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4867145&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