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

Other names:	Etiocholan-3«alpha»-ol-17-one, trimethylsilyl ether
	5«beta»-Androstan-17-one, 3«beta»-(trimethylsiloxy)-
	3«beta»-Trimethylsilyloxy-5«beta»-androstan-17-one
	3-[(Trimethylsilyl)oxy]androstan-17-one, (3«beta»,5«beta»)-
	3«beta»-Hydroxy-5«beta»-androstan-17-one, TMS
	3B-Hydroxy-5B-androstan-17-one, TMS
	Ethiocholan-3«alpha»-ol-17-one, trimethylsilyl ether
	5«BETA»-androstan-3«beta»-ol-17-one, 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-SSLWXMMXSA-N
Formula:	C22H38O2Si
SMILES:	CC12CCC3C(CCC4CC(O[Si](C)(C)C)CCC43C)C1CCC2=O
Mol. weight [g/mol]:	362.62
CAS:	10426-96-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.69		Crippen Method
logp	5.818		Crippen Method
rinpol	2495.00		NIST Webbook
rinpol	2574.50		NIST Webbook
rinpol	2495.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10426967&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

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