

o-Tetramethylen(tert-butyl)silylepiandrosterone

Other names:	3-[(1-tert-Butyl-1-silolanyl)oxy]androstan-17-one-, (3«beta»,5«alpha»)-Epiandrosterone, TMTBSi (3-O)
Inchi:	InChI=1S/C27H46O2Si/c1-25(2,3)30(16-6-7-17-30)29-20-12-14-26(4)19(18-20)8-9-21-22
InchiKey:	BSVQVMAFWBNYSZ-SPKVWTJFSA-N
Formula:	C27H46O2Si
SMILES:	CC12CCC3C(CCC4CC(O[Si]5(C(C)(C)C)CCCC5)CCC43C)C1CCC2=O
Mol. weight [g/mol]:	430.74
CAS:	64898-16-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.68		Crippen Method
logp	7.523		Crippen Method
rinpol	3113.00		NIST Webbook
rinpol	3176.00		NIST Webbook
rinpol	3113.00		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=C64898164&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/49-450-8/o-Tetramethylen-tert-butyl-silylepiandrosterone.pdf>

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