

Androst-4-en-3-one, 17-[(trimethylsilyl)oxy]-, (17«alpha»)-

Other names:

Epitestosterone, o-trimethylsilyl-
4-Androsten-3-one, 17«alpha»-trimethylsilyloxy
17-[(Trimethylsilyl)oxy]androst-4-en-3-one-, (17«alpha»)-
Androst-4-en-17«alpha»-ol-3-one, TMS
Epitestosterone, TMS
Epitestosterone, trimethylsilyl ether
Epitestosterone, per-TMS
Testosterone, 17-TMS
Epitestosterone, tms derivative

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

InchiKey: HNZDTAXZHUIDTM-CEXYIDGCSA-N

Formula: C22H36O2Si

SMILES: CC12CCC(=O)C=C1CCC1C2CCC2(C)C(O[Si](C)(C)C)CCC12

Mol. weight [g/mol]: 360.61

CAS: 16134-45-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.79		Crippen Method
logp	5.738		Crippen Method
rinpol	2675.80		NIST Webbook
rinpol	2667.00		NIST Webbook
rinpol	2645.00		NIST Webbook
rinpol	2652.00		NIST Webbook
rinpol	2645.00		NIST Webbook
rinpol	2667.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C16134455&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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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