4-Androsten-17«alpha»-ol-3-one (epitestosterone), MO-TMS

Inchi: InChI=1S/C23H39NO2Si/c1-22-13-11-17(24-25-3)15-16(22)7-8-18-19-9-10-21(26-27(4,5

InchiKey: SFXUCUOVEDBETC-DSJBWLRPSA-N

Formula: C23H39NO2Si

SMILES: CON=C1C=C2CCC3C(CCC4(C)C(O[Si](C)(C)C)CCC34)C2(C)CC1

Mol. weight [g/mol]: 389.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.17		Crippen Method
logp	6.172		Crippen Method
rinpol	2600.00		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=R523138&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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