

5-«alpha»,16-Androsten-3-one, TMS

Inchi: InChI=1S/C22H36OSi/c1-21-12-6-7-19(21)18-9-8-16-15-17(23-24(3,4)5)10-14-22(16,2)2
InchiKey: PGFCKMIUNGHURL-ZSFLQZPOSA-N
Formula: C22H36OSi
SMILES: CC12C=CCC1C1CCC3CC(O[Si](C)(C)C)=CCC3(C)C1CC2
Mol. weight [g/mol]: 344.61

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.50		Crippen Method
logp	6.540		Crippen Method
rinpol	2155.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R149681&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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