

Androst-5-en-17-one, 3,16-bis[(trimethylsilyl)oxy]-, (3«beta»,16«beta»)-

Other names: Bis(trimethylsilyl) derivative of 16«beta»-Hydroxydehydroepiandrosterone
(3«beta»,16«beta»)-dihydroxy-5-androsten-17-one, TMS

Inchi: InChI=1S/C25H44O3Si2/c1-24-13-11-18(27-29(3,4)5)15-17(24)9-10-19-20(24)12-14-25(

InchiKey: BDPGVCUMZYXUEQ-HYVQQOEGSA-N

Formula: C25H44O3Si2

SMILES: CC12CCC3C(CC=C4CC(O[Si](C)(C)C)CCC43C)C1CC(O[Si](C)(C)C)C2=O

Mol. weight [g/mol]: 448.79

CAS: 40822-67-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.29		Crippen Method
logp	6.568		Crippen Method
rinpol	2727.00		NIST Webbook
rinpol	2729.00		NIST Webbook
rinpol	2698.00		NIST Webbook
rinpol	2698.00		NIST Webbook
rinpol	2727.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C40822671&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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