

Silane, **[[3«beta»,5«alpha»)-androstan-3-yl]oxy]trimethyl**

Other names:

5«alpha»-Androstane, 3«beta»-(trimethylsiloxy)-

Androstane, silane deriv.

3-[(Trimethylsilyl)oxy]androstane

5-«alpha»-Androstan-3-«beta»-ol, TMS

Androstan-3-ol, (3«beta»,5«alpha»)-, tms derivative

Inchi: InChI=1S/C22H40OSi/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: XQQDDEIBTCOQHD-UHFFFAOYSA-N

Formula: C22H40OSi

SMILES: CC12CCCC1C1CCC3CC(O[Si](C)(C)C)CCC3(C)C1CC2

Mol. weight [g/mol]: 348.64

CAS: 18899-44-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.41		Crippen Method
logp	6.639		Crippen Method
rinpol	2275.00		NIST Webbook
rinpol	2295.00		NIST Webbook
rinpol	2285.00		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=C18899440&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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