

3,17-Bis[(trimethylsilyl)oxy]-5«beta»-androstandiol, (3«beta»,17«beta»)-

Other names: 5«beta»-Androstandiol-3«beta»,17«beta»-diol bis(trimethylsilyl) deriv.

5-«beta»-Androstandiol-3-«beta»,17-«beta»-diol, (2TMS)

5«beta»-Androstandiol-3«beta»,17«beta», bis-TMS

5-«beta»-Androstandiol-3-«beta»,17-«beta»-diol, TMS

Androstandiol-3,17-diols, (3«beta»,5«beta»,17«beta»)-, 2tms derivative

Inchi: InChI=1S/C25H48O2Si2/c1-24-15-13-19(26-28(3,4)5)17-18(24)9-10-20-21-11-12-23(27-

InchiKey: KBSHKNYEUGMMDQ-PFDHWQDWSA-N

Formula: C25H48O2Si2

SMILES: CC12CCC(O[Si](C)(C)C)CC1CCC1C2CCC2(C)C(O[Si](C)(C)C)CCC12

Mol. weight [g/mol]: 436.82

CAS: 18880-48-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.92		Crippen Method
logp	7.469		Crippen Method
rinpol	2545.00		NIST Webbook
rinpol	2570.00		NIST Webbook
rinpol	2560.00		NIST Webbook
rinpol	2571.00		NIST Webbook
rinpol	2560.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C18880483&Units=SI>

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

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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