

Silane, [(3«alpha»,5«beta»,17«beta»)-androstane-3,17-diyl]bis(oxy)]bis*(1,1-dimethylethyl)dimethylammonium salt

Other names:

Silane, [(3«alpha»,5«beta»,17«beta»)-androstane-3,17-diyl]bis(oxy)]bis*(1,1-dimethylethyl)dimethylammonium salt
Androstane, silane deriv.

3-«alpha»,17-«beta»-Bis(tert-butyldimethylsilyloxy)-5-«beta»-androstane

5«beta»-Androstan-3«alpha»,17«beta»-diol, TBDMS

Inchi: InChI=1S/C31H60O2Si2/c1-28(2,3)34(9,10)32-23-17-19-30(7)22(21-23)13-14-24-25-15-

InchiKey: VXQXLCZNGSUBJR-OZQFXDJWSA-N

Formula: C31H60O2Si2

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

Mol. weight [g/mol]: 520.98

CAS: 65598-75-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.43		Crippen Method
logp	9.810		Crippen Method
rinpol	3036.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C65598756&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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