17«beta»-Estradiol, 3,17-di(dimethyl-tert-butylsilyl)ether

Other names: 3,17-Bis([tert-butyl(dimethyl)silyl]oxy)estra-1,3,5(10)-triene, (17«beta»)-
«beta»-Estradiol, bis(tert-butyldimethylsilyl) ether
17«beta»-Estradiol, bis-TBDMS
17«beta»-Estradiol, TBDMS
17«BETA»-estradiol, 2tbdms derivative

Inchi: InChI=1S/C30H52O2Si2/c1-28(2,3)33(8,9)31-22-13-15-23-21(20-22)12-14-25-24(23)18-

InchiKey: JFLALYDXWVIVJI-CKMKPYADSA-N

Formula: C30H52O2Si2

SMILES: CC12CCC3c4ccc(O[Si](C)(C)C(C)(C)C)cc4CCC3C1CCC2O[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]: 500.90

CAS: 57711-41-8

Physical Properties

Property code	Value	Unit	Source
ie	7.84	eV	Cheméo Relay (1.0)
log10ws	-7.27		Cheméo Relay (1.0)
logp	9.317		Crippen Method
rinpol	3244.00		NIST Webbook
rinpol	3244.00		NIST Webbook
tf	405.15	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C57711418&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point