2,3,17-Tris[(trimethylsilyl)oxy]estra-1,3,5(10)-trien-(17«beta»)-

Other names: Silane, [[(17«beta»)-estra-1,3,5(10)-triene-2,3,17-triyl]tris(oxy)]tris[trimethyl-
2-Hydroxyoestradiol, tris-TMS
2-Hydroxyoestradiol, TMS
2-Hydroxyestradiol, 3tms derivative

Inchi: InChI=1S/C27H48O3Si3/c1-27-16-15-20-21(23(27)13-14-26(27)30-33(8,9)10)12-11-19-1

InchiKey: GQGHMPHCNWCYQG-VYLCANEFSA-N

Formula: C27H48O3Si3

SMILES: CC12CCC3c4cc(O[Si](C)(C)C)c(O[Si](C)(C)C)cc4CCC3C1CCC2O[Si](C)(C)C

Mol. weight [g/mol]: 504.92

CAS: 51497-42-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.61		Cheméo Relay (1.0)
logp	8.190		Crippen Method
rinpol	2812.00		NIST Webbook
rinpol	2812.00		NIST Webbook
tf	388.49	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C51497428&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):

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

tf: Normal melting (fusion) point