

Bis(trimethylsilyl)estradiol

Other names:	Silane, [[(17«beta»)-estra-1,3,5(10)-triene-3,17-diy]]bis(oxy)]bis[trimethyl- Silane, (estra-1,3,5(10)-trien-3,17«beta»-ylenedioxy)bis[trimethyl- 3,17-Bis[(trimethylsilyl)oxy]estra-1,3,5(10)-triene «beta»-Estradiol, bis(trimethylsilyl) ether Estradiol, 2TMS Oestradiol, bis-TMS Estradiol, TMS Oestradiol, TMS Estradiol, MO TMS Estradiol, 2tms derivative
Inchi:	InChI=1S/C24H40O2Si2/c1-24-15-14-20-19-11-9-18(25-27(2,3)4)16-17(19)8-10-21(20)2
InchiKey:	WJUOLKZHWTVGC-XCBYWJNASA-N
Formula:	C24H40O2Si2
SMILES:	CC12CCC3c4ccc(O[Si](C)(C)C)cc4CCC3C1CCC2O[Si](C)(C)C
Mol. weight [g/mol]:	416.74
CAS:	5150-62-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.86		Crippen Method
logp	6.976		Crippen Method
rinpol	2629.00		NIST Webbook
rinpol	2671.00		NIST Webbook
rinpol	2687.00		NIST Webbook
rinpol	2660.00		NIST Webbook
rinpol	2660.00		NIST Webbook
rinpol	2629.00		NIST Webbook
rinpol	2629.00		NIST Webbook
rinpol	2695.60		NIST Webbook
rinpol	2679.00		NIST Webbook
rinpol	2691.00		NIST Webbook
rinpol	2660.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C5150629&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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<https://www.chemeo.com/cid/30-608-3/Bis-trimethylsilyl-estradiol.pdf>

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