

Tri(trimethylsilyl) derivative of estriol

Other names:	Estratriol tri-TMS Trimethylsilyl ether of estriol Silane, [[16«alpha»,17«beta»]-estra-1,3,5(10)-triene-3,16,17-triyl]tris(oxy)tris(trimethyl- 5,16,17-tris[(trimethylsilyl)oxy]estra-1,3,5(10)-triene, (16«alpha»,17«beta»)- Estriol, tris-TMS Estriol, tris-TMS ether Estriol, tris(trimethylsilyl) ether Oestriol, tris-TMS Tris(trimethylsilyl)estriol Estriol, TMS Oestriol, TMS Estriol, MO TMS Estriol, 3tms derivative
Inchi:	InChI=1S/C27H48O3Si3/c1-27-16-15-22-21-14-12-20(28-31(2,3)4)17-19(21)11-13-23(22
InchiKey:	MCKRDIGCTGOZEH-YHZIIQIWSA-N
Formula:	C27H48O3Si3
SMILES:	CC12CCC3c4ccc(O[Si](C)(C)C)cc4CCC3C1CC(O[Si](C)(C)C)C2O[Si](C)(C)C
Mol. weight [g/mol]:	504.92
CAS:	18888-17-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.37		Crippen Method
logp	7.806		Crippen Method
rinpol	2870.00		NIST Webbook
rinpol	2870.00		NIST Webbook
rinpol	2870.00		NIST Webbook
rinpol	2870.00		NIST Webbook
rinpol	2918.70		NIST Webbook
rinpol	2892.00		NIST Webbook
rinpol	2901.00		NIST Webbook
rinpol	2850.00		NIST Webbook
rinpol	2904.00		NIST Webbook
rinpol	2889.00		NIST Webbook
rinpol	2865.00		NIST Webbook
rinpol	2874.00		NIST Webbook
rinpol	2877.00		NIST Webbook

rinpol	2885.00	NIST Webbook
rinpol	2918.70	NIST Webbook
rinpol	2870.00	NIST Webbook
rinpol	2889.00	NIST Webbook
rinpol	2894.00	NIST Webbook
rinpol	2885.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18888170&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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/29-857-9/Tri-trimethylsilyl-derivative-of-estriol.pdf>

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