Bis(trimethylsilyl)estradiol

Other names:	Silane, [[(17«beta»)-estra-1,3,5(10)-triene-3,17-diyl]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:	WJUROLKZHWTVGC-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
ie	8.38	eV	Cheméo Relay (1.0)
log10ws	-6.26		Cheméo Relay (1.0)
logp	6.976		Crippen Method
rinpol	2687.00		NIST Webbook
rinpol	2660.00		NIST Webbook
rinpol	2671.00		NIST Webbook
rinpol	2660.00		NIST Webbook
rinpol	2629.00		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
tf	372.38	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5150629&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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