Estra-1,3,5(10)-trien-17-one, 3-[(trimethylsilyl)oxy]-

Other names: Estra-1,3,5(10)-trien-17-one, 3-[(trimethylsilyl)oxy]-
Estra-1,3,5(10)-trien-17-one, 3-(trimethylsiloxy)-
Estrone trimethylsilyl ether
Estrone-TMS ether
Oestrone, TMS
Estrone, tms derivative

Inchi: InChI=1S/C21H30O2Si/c1-21-12-11-17-16-8-6-15(23-24(2,3)4)13-14(16)5-7-18(17)19(21

InchiKey: FRJOUBWXHQBBER-UHFFFAOYSA-N

Formula: C21H30O2Si

SMILES: CC12CCC3c4ccc(O[Si](C)(C)C)cc4CCC3C1CCC2=O

Mol. weight [g/mol]: 342.55

Physical Properties

Property code	Value	Unit	Source
ie	8.26	eV	Cheméo Relay (1.0)
log10ws	-5.41		Cheméo Relay (1.0)
logp	5.325		Crippen Method
rinpol	2532.00		NIST Webbook
rinpol	2535.00		NIST Webbook
rinpol	2535.00		NIST Webbook
tf	407.33	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=C1839549&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