

Estra-1,3,5(10),6-tetraen-17-one, 3-[(trimethylsilyl)oxy]-

Other names:	Oestrone, 6-dehydro, TMS
Inchi:	InChI=1S/C21H28O2Si/c1-21-12-11-17-16-8-6-15(23-24(2,3)4)13-14(16)5-7-18(17)19(21)
InchiKey:	BRIXPURCIVSCJA-CTAFRAEOSA-N
Formula:	C21H28O2Si
SMILES:	CC12CCC3c4ccc(O[Si](C)(C)C)cc4C=CC3C1CCC2=O
Mol. weight [g/mol]:	340.53
CAS:	69688-26-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.66		Crippen Method
logp	5.406		Crippen Method
rinpol	2542.00		NIST Webbook
rinpol	2633.00		NIST Webbook
rinpol	2542.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C69688262&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

Latest version available from:

<https://www.chemeo.com/cid/84-752-4/Estra-1-3-5-10-6-tetraen-17-one-3-trimethylsilyl-oxy.pdf>

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