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

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