

1,3,5(10)-Oestratriene-3,17«beta»-diol, 3-TMS-17-PFP

Inchi:	InChI=1S/C24H31F5O3Si/c1-22-12-11-17-16-8-6-15(32-33(2,3)4)13-14(16)5-7-18(17)19
InchiKey:	LXJLIBRGDLFGF-UDGWLPKNSA-N
Formula:	C24H31F5O3Si
SMILES:	CC12CCC3c4ccc(O[Si](C)(C)C)cc4CCC3C1CCC2OC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	490.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.56		Crippen Method
logp	6.866		Crippen Method
rinpol	2551.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R537261&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

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