

# 1,3,5(10)-Oestratriene-3,17«alpha»-diol, 3-TMS-17-HFB

<b>Inchi:</b>	InChI=1S/C25H31F7O3Si/c1-22-12-11-17-16-8-6-15(35-36(2,3)4)13-14(16)5-7-18(17)19
<b>InchiKey:</b>	SKCZEAZINGMGHC-SXFAUFNYSА-N
<b>Formula:</b>	C25H31F7O3Si
<b>SMILES:</b>	CC12CCC3c4ccc(O[Si](C)(C)C)cc4CCC3C1CCC2OC(=O)C(F)(F)C(F)(F)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	540.59

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.30		Crippen Method
logp	7.501		Crippen Method
rinpol	2525.00		NIST Webbook
rinpol	2525.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R537216&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R537216&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## Legend

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

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