

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

Inchi: 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
InchiKey: SKCZEAZINGMGHC-UDGWLPKNSA-N
Formula: C25H31F7O3Si
SMILES: CC12CCC3c4ccc(O[Si](C)(C)C)cc4CCC3C1CCC2OC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 540.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.30		Crippen Method
logp	7.501		Crippen Method
rinpol	2593.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R537256&Units=SI>

Legend

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

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