

1,3,5(10)-Oestratriene-2-methoxy-3,17«beta»-diol, 3-TMS-17-HFB

InChI: COc1cc2c(cc1O[Si](C)(C)C)CCC1C2CCC2(C)C(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)CCC12
InchiKey: IYAZYUBXQIGZGF-IGRNSJNGSA-N
Formula: C₂₆H₃₃F₇O₄Si
SMILES: COc1cc2c(cc1O[Si](C)(C)C)CCC1C2CCC2(C)C(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)CCC12
Mol. weight [g/mol]: 570.61

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.42		Crippen Method
logp	7.510		Crippen Method
rinpol	2718.00		NIST Webbook
rinpol	2718.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R537192&Units=SI>

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/68-337-3/1-3-5-10-Oestratriene-2-methoxy-3-17-beta-diol-3-TMS-17-HFB.pdf>

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