

# 1,3,5(10)-Oestratriene-2-methoxy-3,16«alpha»,17«beta»-triol-3-TBDMS-16,17-TFA

InChI: COc1cc2c(cc1O[Si](C)(C)C(C)(C)C)CCC1C2CCC2(C)C1CC(OC(=O)C(F)(F)F)C2OC(=O)C(F)(F)F  
InchiKey: ROZNEEBOYMMKNK-HCVCXDRWSA-N

Formula:

C<sub>29</sub>H<sub>38</sub>F<sub>6</sub>O<sub>6</sub>Si

SMILES:

COc1cc2c(cc1O[Si](C)(C)C(C)(C)C)CCC1C2CCC2(C)C1CC(OC(=O)C(F)(F)F)C2OC(=O)C(F)(F)F

Mol. weight [g/mol]:

624.68

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.68		Crippen Method
logp	7.493		Crippen Method
rinpol	2808.00		NIST Webbook
rinpol	2808.00		NIST Webbook

## Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R537167&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/67-679-5/1-3-5-10-Oestratriene-2-methoxy-3-16-alpha-17-beta-triol-3-TBDMS-16-17-TFA>

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