1,3,5(10)-Oestratriene-3,17«alpha»-diol, 3-TBDMS-17-PFP

Inchi: InChI=1S/C27H37F5O3Si/c1-24(2,3)36(5,6)35-17-8-10-18-16(15-17)7-9-20-19(18)13-14-

InchiKey: GYEMEQOWYBXDGA-CZLVRFMKSA-N

Formula: C27H37F5O3Si

SMILES: CC12CCC3c4ccc(O[Si](C)(C)C(C)(C)C)cc4CCC3C1CCC2OC(=O)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 532.66

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.70		Cheméo Relay (1.0)
logp	8.036		Crippen Method
rinpol	2757.00		NIST Webbook
rinpol	2757.00		NIST Webbook
tf	384.64	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R537201&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

tf: Normal melting (fusion) point

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