1,3,5(10)-Oestratriene-3,17.beta.-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-QBSOXGLUSA-N

Formula: C27H37F5O3Si

SMILES: CC(C)(C)[Si](C)(C)Oc1ccc2c(c1)CC[C@@H]1[C@@H]2CC[C@]2(C)[C@@H](OC(=O)C

Mol. weight [g/mol]: 532.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.72		Cheméo Relay (1.0)
logp	8.036		Crippen Method
tf	408.76	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?Str2File=R537241

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

tf: Normal melting (fusion) point