

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

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