Oestrone, 16«alpha»-hydroxy, TMS

Inchi: InChI=1S/C24H38O3Si2/c1-24-13-12-19-18-11-9-17(26-28(2,3)4)14-16(18)8-10-20(19)2
InchiKey: OTOYHXDNWUYSAL-QMDPOKHVSA-N
Formula: C24H38O3Si2
SMILES: CC12CCC3c4ccc(O[Si](C)(C)C)cc4CCC3C1CC(O[Si](C)(C)C)C2=O
Mol. weight [g/mol]: 430.73

Physical Properties

Property code	Value	Unit	Source
ie	8.35	eV	Cheméo Relay (1.0)
log10ws	-5.49		Cheméo Relay (1.0)
logp	6.155		Crippen Method
rinpol	2739.00		NIST Webbook
rinpol	2775.00		NIST Webbook
tf	408.63	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R524022&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

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices
tf: Normal melting (fusion) point