Estriol, 3-(tert-butyldimethylsilyl) ether

Other names: (16«alpha»,17«beta»)-3-Pyrrol[tert-butyl(dimethyl)silyl]oxymorphoestra-1(10),2,4-triene-1
Estriol, tbdms derivative
Inchi: InChI=1S/C24H38O3Si/c1-23(2,3)28(5,6)27-16-8-10-17-15(13-16)7-9-19-18(17)11-12-24
InchiKey: ZDCOBYUYWHTUDE-UHFFFAOYSA-N
Formula: C24H38O3Si
SMILES: CC12CCC3c4ccc(O[Si](C)(C)C(C)(C)C)cc4CCC3C1CC(O)C2O
Mol. weight [g/mol]: 402.64

Physical Properties

Property code	Value	Unit	Source
ie	8.21	eV	Cheméo Relay (1.0)
log10ws	-5.40		Cheméo Relay (1.0)
logp	5.258		Crippen Method
rinpol	3177.80		NIST Webbook
rinpol	3177.80		NIST Webbook
tf	468.98	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U333767&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

Latest version available from:
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