17-epi-Oestriol, TMS

Inchi: InChI=1S/C24H40O2Si2/c1-24-15-14-20-19-11-9-18(25-27(2,3)4)16-17(19)8-10-21(20)2
InchiKey: WJUROLKZHWTVGC-QGOPKKHISA-N
Formula: C24H40O2Si2
SMILES: CC12CCC3c4ccc(O[Si](C)(C)C)cc4CCC3C1CCC2O[Si](C)(C)C
Mol. weight [g/mol]: 416.74

Physical Properties

Property code	Value	Unit	Source
ie	8.38	eV	Cheméo Relay (1.0)
log10ws	-6.26		Cheméo Relay (1.0)
logp	6.976		Crippen Method
rinpol	2855.00		NIST Webbook
rinpol	2853.00		NIST Webbook
rinpol	2868.00		NIST Webbook
rinpol	2855.00		NIST Webbook
rinpol	2853.00		NIST Webbook
tf	372.38	K	Cheméo Relay (1.0)

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R166280&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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