

17«beta»-Oestradiol, TMS

Other names: 17«beta»-Estradiol, 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-RNFCRKIASA-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
log10ws	-2.86		Crippen Method
logp	6.976		Crippen Method
rinpol	2616.00		NIST Webbook
rinpol	2683.00		NIST Webbook
rinpol	2634.00		NIST Webbook
rinpol	2653.00		NIST Webbook
rinpol	2616.00		NIST Webbook
rinpol	2634.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R523930&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/46-115-3/17-beta-Oestradiol-TMS.pdf>

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