5«alpha»-Estranediol-3«alpha»,17«beta», bis-TMS

Inchi: InChI=1S/C24H46O2Si2/c1-24-15-14-20-19-11-9-18(25-27(2,3)4)16-17(19)8-10-21(20)2

InchiKey: UOQHQBNVJDUSEX-DMGKZOFXSA-N

Formula: C24H46O2Si2

SMILES: CC12CCC3C4CCC(O[Si](C)(C)C)CC4CCC3C1CCC2O[Si](C)(C)C

Mol. weight [g/mol]: 422.79

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.50		Crippen Method
logp	7.079		Crippen Method
rinpol	2491.00		NIST Webbook
rinpol	2502.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R297700&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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https://www.chemeo.com/cid/54-564-6/5-alpha-Estranediol-3-alpha-17-beta-bis-TMS.pdf

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