

3«beta»-Hydroxy-5«alpha»-estran-16-one, TMS

Inchi: InChI=1S/C21H36O2Si/c1-21-10-9-18-17-8-6-16(23-24(2,3)4)11-14(17)5-7-19(18)20(21)
InchiKey: INGPVCGBLYBUNV-DJDYUMQYSA-N
Formula: C21H36O2Si
SMILES: CC12CCC3C4CCC(O[Si](C)(C)C)CC4CCC3C1CC(=O)C2
Mol. weight [g/mol]: 348.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.27		Crippen Method
logp	5.428		Crippen Method
rinpol	2435.00		NIST Webbook
rinpol	2530.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R523965&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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.chemeo.com/cid/65-585-1/3-beta-Hydroxy-5-alpha-estran-16-one-TMS.pdf>

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