

15(ksi)-Hydroxyoestriol, TMS

Inchi: InChI=1S/C30H56O4Si4/c1-30-19-18-24-23-17-15-22(31-35(2,3)4)20-21(23)14-16-25(24)
InchiKey: RSQDODOMVGFYEA-SUCWCPSBSA-N
Formula: C30H56O4Si4
SMILES: CC12CCC3c4ccc(O[Si](C)(C)C)cc4CCC3C1C(O[Si](C)(C)C)C(O[Si](C)(C)C)C2O[Si](C)(C)C
Mol. weight [g/mol]: 593.11

Physical Properties

Property code	Value	Unit	Source
log10ws	0.13		Crippen Method
logp	8.636		Crippen Method
rinpol	3076.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R166191&Units=SI>

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/29-972-1/15-ksi-Hydroxyoestriol-TMS.pdf>

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