

11B-Hydroxyoestradiol, TMS

Inchi: InChI=1S/C27H48O3Si3/c1-27-18-24(29-32(5,6)7)26-21-14-12-20(28-31(2,3)4)17-19(21)
InchiKey: LCDDQBUJLDWLBA-MMZAQROYSA-N
Formula: C27H48O3Si3
SMILES: CC12CC(O[Si](C)(C)C)C3c4ccc(O[Si](C)(C)C)cc4CCC3C1CCC2O[Si](C)(C)C
Mol. weight [g/mol]: 504.92

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.37		Crippen Method
logp	7.806		Crippen Method
rinpol	2809.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R166166&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/17-065-1/11B-Hydroxyoestradiol-TMS.pdf>

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