

11-Ketoestradiol (enol), TMS

Inchi: InChI=1S/C27H46O3Si3/c1-27-18-24(29-32(5,6)7)26-21-14-12-20(28-31(2,3)4)17-19(21)
InchiKey: PPBFFDCVRWUUNH-ORLBZUTRSA-N
Formula: C27H46O3Si3
SMILES: CC12C=C(O[Si](C)(C)C)C3c4ccc(O[Si](C)(C)C)cc4CCC3C1CCC2O[Si](C)(C)C
Mol. weight [g/mol]: 502.91

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.61		Crippen Method
logp	7.932		Crippen Method
rinpol	2903.00		NIST Webbook
rinpol	2906.00		NIST Webbook
rinpol	2903.00		NIST Webbook

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=R166304&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/47-999-2/11-Ketoestradiol-enol-TMS.pdf>

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