

4-Hydroxyoestrone (enol), TMS

Inchi: InChI=1S/C27H46O3Si3/c1-27-18-17-20-19-13-15-24(28-31(2,3)4)26(30-33(8,9)10)22(11,12)32
InchiKey: BBVVKMKFKXGUEL-ISINKVRMSA-N
Formula: C27H46O3Si3
SMILES: CC12CCC3c4ccc(O[Si](C)(C)C)c(O[Si](C)(C)C)c4CCC3C1CC=C2O[Si](C)(C)C
Mol. weight [g/mol]: 502.91

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.11		Crippen Method
logp	8.315		Crippen Method
rinpol	2789.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R166384&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.cheméo.com/cid/31-896-3/4-Hydroxyoestrone-enol-TMS.pdf>

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