

2-Hydroxyoestrone (enol), TMS

Inchi: InChI=1S/C27H46O3Si3/c1-27-16-15-20-21(23(27)13-14-26(27)30-33(8,9)10)12-11-19-1
InchiKey: ARHVAJXLYBXHBH-ISINKVRMSA-N
Formula: C27H46O3Si3
SMILES: CC12CCC3c4cc(O[Si](C)(C)C)c(O[Si](C)(C)C)cc4CCC3C1CC=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	2772.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R166339&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/57-027-9/2-Hydroxyoestrone-enol-TMS.pdf>

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