

18-Hydroxyoestrone (enol), TMS

Inchi: InChI=1S/C27H46O3Si3/c1-31(2,3)28-19-27-17-16-23-22-13-11-21(29-32(4,5)6)18-20(2)
InchiKey: CYEPVODJXIMLIK-ZXICVGLGSA-N
Formula: C27H46O3Si3
SMILES: C[Si](C)(C)OCC12CCC3c4ccc(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	-1.49		Crippen Method
logp	7.933		Crippen Method
rinpol	2815.00		NIST Webbook
rinpol	2815.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R166295&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/29-867-8/18-Hydroxyoestrone-enol-TMS.pdf>

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