

11-Dehydroestrone (enol), TMS

Inchi: InChI=1S/C24H36O2Si2/c1-24-15-14-20-19-11-9-18(25-27(2,3)4)16-17(19)8-10-21(20)2
InchiKey: RTPDSJWDENKOGH-XRCKSUEFSA-N
Formula: C24H36O2Si2
SMILES: CC12C=CC3c4ccc(O[Si](C)(C)C)cc4CCC3C1CC=C2O[Si](C)(C)C
Mol. weight [g/mol]: 412.71

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.95		Crippen Method
logp	6.878		Crippen Method
rinpol	2783.00		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=R166097&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/44-282-0/11-Dehydroestrone-enol-TMS.pdf>

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