11-Dehydroestradiol, TMS

Inchi:	InChI=1S/C24H38O2Si2/c1-24-15-14-20-19-11-9-18(25-27(2,3)4)16-17(19)8-10-21(20)2
InchiKey:	FXHWAZNSHXQSOJ-WQABULOPSA-N
Formula:	C24H38O2Si2
SMILES:	CC12C=CC3c4ccc(O[Si](C)(C)C)cc4CCC3C1CCC2O[Si](C)(C)C
Mol. weight [g/mol]:	414.73

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.72		Crippen Method
logp	6.752		Crippen Method
rinpol	2549.00		NIST Webbook
rinpol	2549.00		NIST Webbook
rinpol	2549.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R166077&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/12-873-9/11-Dehydroestradiol-TMS.pdf
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