

5-Pregnen-3-«beta»,15-«beta»,17-«alpha»,20-«alpha»-TMS

Other names:	5-Pregnen-3-«beta»,15-«beta»,17-«alpha»,20-«alpha»-tetrol, MeTMS
Inchi:	InChI=1S/C33H66O4Si4/c1-24(34-38(4,5)6)33(37-41(13,14)15)23-29(36-40(10,11)12)30
InchiKey:	ISLSOODKDGSAJC-RYQWTPGRSA-N
Formula:	C33H66O4Si4
SMILES:	CC(O[Si](C)(C)C)C1(O[Si](C)(C)C)CC(O[Si](C)(C)C)C2C3CC=C4CC(O[Si](C)(C)C)CCC
Mol. weight [g/mol]:	639.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.86		Crippen Method
logp	9.830		Crippen Method
rinpol	3058.00		NIST Webbook
rinpol	3058.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R393536&Units=SI

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/56-565-3/5-Pregnen-3-beta-15-beta-17-alpha-20-alpha-tetrol-TMS.pdf>

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