

5-«alpha»-Pregnan-3-«beta»-ol-11-one, MO-TMS

Inchi:	InChI=1S/C25H45NO2Si/c1-8-17-10-12-21-20-11-9-18-15-19(28-29(5,6)7)13-14-24(18,2
InchiKey:	IFKSNQUFNAHUPS-PGLLCUAGSA-N
Formula:	C25H45NO2Si
SMILES:	CCC1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3C(=NOC)CC12C
Mol. weight [g/mol]:	419.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.67		Crippen Method
logp	6.888		Crippen Method
rinpol	2663.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R486707&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

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<https://www.chemeo.com/cid/35-843-7/5-alpha-Pregnan-3-beta-ol-11-one-MO-TMS.pdf>

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