

5-«beta»-Pregnan-20-«beta»-ol-11-one, MO-TMS

Inchi:	InChI=1S/C25H45NO2Si/c1-17(28-29(5,6)7)20-13-14-21-19-12-11-18-10-8-9-15-24(18,2
InchiKey:	AENBXJWUEFXGGT-YXKFZKHVSA-N
Formula:	C25H45NO2Si
SMILES:	CON=C1CC2(C)C(C(C)O[Si](C)(C)C)CCC2C2CCC3CCCCC3(C)C12
Mol. weight [g/mol]:	419.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.67		Crippen Method
logp	6.888		Crippen Method
rinpol	2610.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R486861&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/17-533-1/5-beta-Pregnan-20-beta-ol-11-one-MO-TMS.pdf>

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