

5-«beta»-Pregnan-20-«alpha»-ol-3-one, MO-TMS

Inchi:	InChI=1S/C25H45NO2Si/c1-17(28-29(5,6)7)21-10-11-22-20-9-8-18-16-19(26-27-4)12-14
InchiKey:	MEPCJQMOKOWTNN-DWYSCYBMSA-N
Formula:	C25H45NO2Si
SMILES:	CON=C1CCC2(C)C(CCC3C2CCC2(C)C(C(C)O[Si](C)(C)C)CCC32)C1
Mol. weight [g/mol]:	419.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.67		Crippen Method
logp	6.888		Crippen Method
rinpol	2790.00		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=R486841&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/27-970-5/5-beta-Pregnan-20-alpha-ol-3-one-MO-TMS.pdf>

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