

Pregnane-3,20-dione, 11-[(trimethylsilyl)oxy]-, bis(O-methyloxime), (5«beta»,11«beta»)-

Other names:	5-«beta»-Pregnan-11-«beta»-ol-3,20-dione, MO-TMS
Inchi:	InChI=1S/C26H46N2O3Si/c1-17(27-29-4)21-11-12-22-20-10-9-18-15-19(28-30-5)13-14-2
InchiKey:	OIUIKIGMQBHOGH-VUIIBYKFSA-N
Formula:	C26H46N2O3Si
SMILES:	CON=C1CCC2(C)C(CCC3C4CCC(C(C)=NOC)C4(C)CC(O[Si](C)(C)C)C32)C1
Mol. weight [g/mol]:	462.74
CAS:	57305-27-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.33		Crippen Method
logp	6.500		Crippen Method
rinpol	2862.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57305278&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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