

5-«beta»-Pregnan-3-«alpha»-ol-11,20-dione, MO-TMS

Inchi:	InChI=1S/C26H46N2O3Si/c1-17(27-29-4)21-11-12-22-20-10-9-18-15-19(31-32(6,7)8)13-
InchiKey:	QNTUYUZHRGUGNY-LSXSRRAZSA-N
Formula:	C26H46N2O3Si
SMILES:	CON=C(C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3C(=NOC)CC12C
Mol. weight [g/mol]:	462.74

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.33		Crippen Method
logp	6.500		Crippen Method
rinpol	2776.00		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=R487002&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.cheméo.com/cid/53-929-2/5-beta-Pregnan-3-alpha-ol-11-20-dione-MO-TMS.pdf>

Generated by Cheméo on 2024-04-26 14:01:58.396452246 +0000 UTC m=+16429367.317029562.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.