

4-Pregnen-11-«beta»,20-«alpha»-diol-3-one, MO-TMS

Inchi:	InChI=1S/C28H51NO3Si2/c1-19(31-33(5,6)7)23-13-14-24-22-12-11-20-17-21(29-30-4)15
InchiKey:	POLSCKPVKDCQEJ-FBFYOZOESA-N
Formula:	C28H51NO3Si2
SMILES:	CON=C1C=C2CCC3C(C(O[Si](C)(C)C)CC4(C)C(C(C)O[Si](C)(C)C)CCC34)C2(C)CC1
Mol. weight [g/mol]:	505.88

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.27		Crippen Method
logp	7.638		Crippen Method
rinpol	3130.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R486138&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/43-814-0/4-Pregnen-11-beta-20-alpha-diol-3-one-MO-TMS.pdf>

Generated by Cheméo on 2024-04-23 17:34:59.572502657 +0000 UTC m=+16182948.493079968.

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