

Pregn-4-ene-3,20-dione, 6-methyl-17-[(trimethylsilyl)oxy]-, bis(O-methyloxime), (6«alpha»)-

Other names:

6«alpha»-Methyl-17-hydroxyprogesterone, MO-TMS

InChI: InChI=1S/C27H46N2O3Si/c1-18-16-21-22(23(3)13-10-20(29-31-6)17-24(18)25)11-14-26

InchiKey: ZTZGORUGVYGHSD-GCBZSIETSA-N
Formula: C27H46N2O3Si
SMILES: CON=C1C=C2C(C)CC3C(CCC4(C)C3CCC4(O[Si](C)(C)C)C(C)=NOC)C2(C)CC1
Mol. weight [g/mol]: 474.75
CAS: 69833-56-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.84		Crippen Method
logp	6.810		Crippen Method
rinpol	2970.00		NIST Webbook
rinpol	2970.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C69833563&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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