

5«alpha»-Pregnan-20-one, 3«alpha»,17-bis(trimethylsiloxy)-, O-methyl oxime

Other names:

17(5«alpha»)-OH-Pregnanolone, MO-TMS

Inchi:

InChI=1S/C28H53NO3Si2/c1-20(29-30-4)28(32-34(8,9)10)18-15-25-23-12-11-21-19-22(3)

InchiKey:

WPPGDMRLWMCELS-VGSWSJQWSA-N

Formula:

C28H53NO3Si2

SMILES:

CON=C(C)C1(O[Si](C)(C)C)CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC21C

Mol. weight [g/mol]:

507.90

CAS:

33287-42-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.41		Crippen Method
logp	7.862		Crippen Method
rinpol	2766.00		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=C33287422&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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