

5-«alpha»-Pregnan-3-«alpha»,11-«beta»-diol-20-one

MO-TMS

InChIKey:

InChI=1S/C28H53NO3Si2/c1-19(29-30-4)23-13-14-24-22-12-11-20-17-21(31-33(5,6)7)15

Formula:

C28H53NO3Si2

SMILES:

CON=C(C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3C(O[Si](C)(C)C)CC12C

Mol. weight [g/mol]:

507.90

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.17		Crippen Method
logp	7.718		Crippen Method
rinpol	2921.00		NIST Webbook
rinpol	2847.00		NIST Webbook

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R422109&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.chemeo.com/cid/64-483-5/5-alpha-Pregnan-3-alpha-11-beta-diol-20-one-MO-TMS.pdf>

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