

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

MO-TMS

InchiKey:

InChI=1S/C28H53NO3Si2/c1-19(31-33(5,6)7)23-13-14-24-22-12-11-20-17-21(32-34(8,9)

YXNCMXWVSHUSLE-VZWCWSLSA-N

Formula:

C28H53NO3Si2

SMILES:

CON=C1CC2(C)C(C(C)O[Si](C)(C)C)CCC2C2CCC3CC(O[Si](C)(C)C)CCC3(C)C12

Mol. weight [g/mol]:

507.90

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.17		Crippen Method
logp	7.718		Crippen Method
rinpol	2906.00		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R486990&Units=SI>

Crippen Method:

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

Crippen Method:

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

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/36-437-7/5-beta-Pregnan-3-alpha-20-beta-diol-11-one-MO-TMS.pdf>

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