

5«beta»-Pregnane-3«beta»,17«alpha»-diol-20-one

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-GOUXDGQCSA-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

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.41		Crippen Method
logp	7.862		Crippen Method
rinpol	2756.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R250538&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/54-724-8/5-beta-Pregnane-3-beta-17-alpha-diol-20-one-MO-TMS.pdf>

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