

5-«alpha»-Pregnan-3-«beta»-16-«alpha»-diol-20-one-TMS

InChIKey:

InChI=1S/C27H50O3Si2/c1-18(28)25-24(30-32(7,8)9)17-23-21-11-10-19-16-20(29-31(4,5)6)22-26-27-33-34-35-36-37

Formula:

C₂₇H₅₀O₃Si₂

SMILES:

CC(=O)C1C(O[Si](C)(C)C)CC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC21C

Mol. weight [g/mol]:

478.86

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.79		Crippen Method
logp	7.284		Crippen Method
rinpol	2856.00		NIST Webbook
rinpol	2856.00		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R393907&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.cheméo.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.cheméo.com/cid/38-861-4/5-alpha-Pregnan-3-beta-16-alpha-diol-20-one-TMS.pdf>

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