

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

MO-TMS

InChIKey:

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

Formula:

C28H53NO3Si2

SMILES:

CON=C1CCC2(C)C(CCC3C4CCC(C(C)O[Si](C)(C)C)C4(C)CC(O[Si](C)(C)C)C32)C1

Mol. weight [g/mol]:

507.90

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.17		Crippen Method
logp	7.718		Crippen Method
rinpol	3010.00		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R486376&Units=SI>

Crippen Method:

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

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/25-099-5/5-alpha-Pregnan-11-beta-20-beta-diol-3-one-MO-TMS.pdf>

Generated by Cheméo on 2024-04-29 01:11:05.823548178 +0000 UTC m=+16642314.744125495.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.