

4-Pregnen-3-«beta»,20-«alpha»-diol, TMS

Inchi: InChI=1S/C27H50O2Si2/c1-19(28-30(4,5)6)23-12-13-24-22-11-10-20-18-21(29-31(7,8)9)
InchiKey: MCJUHONVKSCXOU-CFEBSQMISA-N
Formula: C27H50O2Si2
SMILES: CC(O[Si](C)(C)C)C1CCC2C3CCC4=CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 462.86

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.61		Crippen Method
logp	8.026		Crippen Method
rinpol	2860.00		NIST Webbook
rinpol	2860.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R486287&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/29-544-6/4-Pregnen-3-beta-20-alpha-diol-TMS.pdf>

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