

5-Pregnen-3-«beta»,11-«beta»-diol, TMS

Inchi: InChI=1S/C27H50O2Si2/c1-10-19-12-14-23-22-13-11-20-17-21(28-30(4,5)6)15-16-26(20)
InchiKey: DXIIMAYVNWGSGX-RMGMAWNNSA-N
Formula: C27H50O2Si2
SMILES: CCC1CCC2C3CC=C4CC(O[Si](C)(C)C)CCC4(C)C3C(O[Si](C)(C)C)CC12C
Mol. weight [g/mol]: 462.86

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.61		Crippen Method
logp	8.026		Crippen Method
rinpol	2718.00		NIST Webbook
rinpol	2718.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R487186&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/67-791-0/5-Pregnen-3-beta-11-beta-diol-TMS.pdf>

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