Pregnenolone, 3-dimethyl(t-butyl)silyl ether

Other names: 5-Pregnen-3«beta»-ol-20-one, TBDMS
Inchi: InChI=1S/C27H46O2Si/c1-18(28)22-11-12-23-21-10-9-19-17-20(29-30(7,8)25(2,3)4)13-1
InchiKey: XMTKPEYPGQAHCU-UHFFFAOYSA-N
Formula: C27H46O2Si
SMILES: CC(=O)C1CCC2C3CC=C4CC(O[Si](C)(C)C(C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 430.74

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.64		Crippen Method
logp	7.545		Crippen Method
rinpol	2975.00		NIST Webbook
rinpol	2975.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U308845&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