5-Pregnen-3«beta»-ol-20-one, tert-butyldimethylsilyl ether

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	-5.78		Cheméo Relay (1.0)
logp	7.545		Crippen Method
rinpol	3048.30		NIST Webbook
tf	414.53	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U352612&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices
tf: Normal melting (fusion) point

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