

5«beta»-Pregnane-3«alpha»,17«alpha»,20«alpha» (3,17-O)-TBDMSi, (20-O)-TMSi

Inchi: CC1(O[Si](C)(C)C(C)C)C1(O[Si](C)(C)C(C)(C)C)CCC2C3CCC4CC(O[Si](C)(C)C(C)(C)C)CCC
InchiKey: ZJXYBJXQKXKRV-ZZNGRRPZSA-N
Formula: C36H72O3Si3
SMILES: CC(O[Si](C)(C)C)C1(O[Si](C)(C)C(C)(C)C)CCC2C3CCC4CC(O[Si](C)(C)C(C)(C)C)CCC
Mol. weight [g/mol]: 637.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.77		Crippen Method
logp	11.420		Crippen Method
rinpol	3317.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R144235&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/42-626-0/5-beta-Pregnane-3-alpha-17-alpha-20-alpha-triol-3-17-O-TBDMSi-20-O-TMSi>

Generated by Cheméo on 2024-04-27 20:51:32.007828138 +0000 UTC m=+16540340.928405459.

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