3«alpha»,7«beta»,17«alpha»-trihydroxy-5«beta»-c
acid, TMS

Inchi: InChI=1S/C36H72O5Si4/c1-26(16-17-32(37)40-44(10,11)12)36(41-45(13,14)15)23-20-30
InchiKey: CQOCBDHGMLOCMN-DIMYLECUSA-N
Formula: C36H72O5Si4
SMILES: CC(CCC(=O)O[Si](C)(C)C)C1(O[Si](C)(C)C)CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C
Mol. weight [g/mol]: 697.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.44		Crippen Method
logp	10.464		Crippen Method
rinpol	3418.00		NIST Webbook
rinpol	3419.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R279955&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

Latest version available from:
https://www.chemeo.com/cid/21-448-1/3-alpha-7-beta-17-alpha-trihydroxy-5-beta-cholan-24-oic-acid-TMS.pdf
Generated by Cheméo on 2024-10-12 04:26:06.11099277 +0000 UTC m=+3288028.747962020.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.