5«beta»-Cholestane-3«alpha»,7«alpha»,12«alpha»-TMS

InChI: InChI=1S/C38H78O4Si4/c1-27(20-22-36(2,3)42-46(15,16)17)30-18-19-31-35-32(26-34(3

InchiKey: CMMPFHDYLIVWHZ-LJFVFAHASA-N

Formula: C38H78O4Si4

SMILES: CC(CCC(C)(C)O[Si](C)(C)C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C

Mol. weight [g/mol]: 711.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.37		Crippen Method
logp	11.572		Crippen Method
rinpol	3447.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R271679&Units=SI

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/47-652-6/5-beta-Cholestane-3-alpha-7-alpha-12-alpha-25-tetrol-TMS.pdf
Generated by Cheméo on 2024-04-23 13:04:03.547976273 +0000 UTC m=+16166692.468553588.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.