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

InChI: InChI=1S/C41H86O5Si5/c1-29(25-36(44-49(12,13)14)39(2,3)46-51(18,19)20)32-21-22-3

InChIKey: OOAPDDQLBPWGEZ-LVKGSJJCSA-N

Formula: C41H86O5Si5

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

Mol. weight [g/mol]: 799.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.88		Crippen Method
logp	12.402		Crippen Method
rinpol	3597.00		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=R271659&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices