5B-Cholestane-3A,7A,25-triol, TMS

Inchi: InChI=1S/C36H72O3Si3/c1-26(16-15-21-34(2,3)39-42(12,13)14)29-17-18-30-33-31(20-2
InchiKey: ZRSIZXDWWKIYHV-BCDXPMNXSA-N
Formula: C36H72O3Si3
SMILES: CC(CCCC(C)(C)O[Si](C)(C)C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C
Mol. weight [g/mol]: 637.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.29		Crippen Method
logp	11.132		Crippen Method
rinpol	3436.00		NIST Webbook
rinpol	3436.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R585196&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices