5-Cholesten-3-«beta»,7-«alpha»,27-triol, TMS

Other names: 5-Cholesten-3-«beta»,7-«alpha»,26-triol, TMS
7«alpha»,27-Dihydroxycholesterol, TMS
Inchi: InChI=1S/C36H70O3Si3/c1-26(25-37-40(5,6)7)15-14-16-27(2)30-17-18-31-34-32(20-22-
InchiKey: OIKRTDOOOQVHEN-CCXVUOGASA-N
Formula: C36H70O3Si3
SMILES: CC(CCCC(C)C1CCC2C3C(O[Si](C)(C)C)C=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C)C
Mol. weight [g/mol]: 635.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.03		Crippen Method
logp	10.909		Crippen Method
rinpol	3429.00		NIST Webbook
rinpol	3432.00		NIST Webbook
rinpol	3445.00		NIST Webbook
rinpol	3445.00		NIST Webbook
rinpol	3429.00		NIST Webbook
rinpol	3432.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R177567&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