5-Cholestenoic acid, 3-«beta»-ol, TMS

Inchi: InChI=1S/C33H60O3Si2/c1-23(12-11-13-24(2)31(34)36-38(8,9)10)28-16-17-29-27-15-14
InchiKey: KFCUEYRSEFZHGW-MTCBLDTQSA-N
Formula: C33H60O3Si2
SMILES: CC(CCCC(C)C1CCC2C3CC=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C)C(=O)O[Si](C)(C
Mol. weight [g/mol]: 561.00

Physical Properties

Property code	Value	Unit	Source
hvap	132.81	kJ/mol	Cheméo Relay (1.0)
log10ws	-7.41		Cheméo Relay (1.0)
logp	9.606		Crippen Method
rinpol	3444.00		NIST Webbook
rinpol	3445.00		NIST Webbook
rinpol	3445.00		NIST Webbook
rinpol	3444.00		NIST Webbook
tb	707.19	K	Cheméo Relay (1.0)
tf	387.59	K	Cheméo Relay (1.0)

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R177636&Units=SI

Legend

hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point