5-Cholesten-3«beta»,7«alpha»-diol, VDMS

Inchi: InChI=1S/C35H62O2Si2/c1-12-38(8,9)36-28-19-21-34(6)27(23-28)24-32(37-39(10,11)13
InchiKey: RMOZJRHDQSUJEX-PSJCLWMVSA-N
Formula: C35H62O2Si2
SMILES: C=C[Si](C)(C)OC1CCC2(C)C(=CC(O[Si](C)(C)C=C)C3C2CCC2(C)C(C(C)CCCC(C)C)CC
Mol. weight [g/mol]: 571.04

Physical Properties

Property code	Value	Unit	Source
hvap	130.62	kJ/mol	Cheméo Relay (1.0)
log10ws	-8.23		Cheméo Relay (1.0)
logp	10.269		Crippen Method
rinpol	3410.00		NIST Webbook
rinpol	3410.00		NIST Webbook
tb	726.30	K	Cheméo Relay (1.0)
tf	353.42	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=R529498&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