5-Cholesten-3.beta.,7.beta.-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-BNNKJLAJSA-N
Formula: C35H62O2Si2
SMILES: C=C[Si](C)(C)O[C@H]1CC[C@@]2(C)C(=C[C@H](O[Si](C)(C)C=C)C3C4CC[C@H]([C@
Mol. weight [g/mol]: 571.05

Physical Properties

Property code	Value	Unit	Source
hvap	113.74	kJ/mol	Cheméo Relay (1.0)
log10ws	-8.29		Cheméo Relay (1.0)
logp	10.269		Crippen Method
tb	722.88	K	Cheméo Relay (1.0)
tf	367.09	K	Cheméo Relay (1.0)

Sources

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?Str2File=R529507
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point

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