3.beta.-hydroxy-5-chol-24-oate, TMS

Inchi: InChI=1S/C30H54O3Si2/c1-21(10-15-28(31)33-35(7,8)9)25-13-14-26-24-12-11-22-20-23
InchiKey: AXHZBMACZNLTNO-WOGDKAGISA-N
Formula: C30H54O3Si2
SMILES: CC(CCC(=O)O[Si](C)(C)C)[C@H]1CCC2C3CC=C4C[C@@H](O[Si](C)(C)C)CC[C@]4(C
Mol. weight [g/mol]: 518.93

Physical Properties

Property code	Value	Unit	Source
hvap	117.88	kJ/mol	Cheméo Relay (1.0)
log10ws	-6.62		Cheméo Relay (1.0)
logp	8.580		Crippen Method
tb	697.61	K	Cheméo Relay (1.0)
tf	392.04	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?Str2File=R492301
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):

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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https://www.chemeo.com/cid/118-842-6/3-beta-hydroxy-5-chol-24-oate-TMS.pdf

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