5«beta»-Cholestane-3«alpha»,7«alpha»-diol, TMS

Inchi: InChI=1S/C32H62O2Si2/c1-22(2)12-13-23(3)26-14-15-27-30-28(17-19-32(26,27)5)31(4)
InchiKey: IFFGLIAZFRHLLK-PRYZTBJMSA-N
Formula: C32H62O2Si2
SMILES: CC(C)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 535.00

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.27		Cheméo Relay (1.0)
logp	9.768		Crippen Method
rinpol	3212.00		NIST Webbook
rinpol	3212.00		NIST Webbook
tf	370.98	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?ID=R271748&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices
tf: Normal melting (fusion) point

Latest version available from:
https://www.chemeo.com/cid/114-017-6/5-beta-Cholestane-3-alpha-7-alpha-diol-TMS.pdf

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