

5«alpha»-cholestan-3«beta»,25-diol, DMESI

Inchi: InChI=1S/C35H68O2Si2/c1-12-38(8,9)36-28-20-23-34(6)27(25-28)16-17-29-31-19-18-30
InchiKey: IQBYEROPYWHVNQ-YWZJEILASA-N
Formula: C35H68O2Si2
SMILES: CC[Si](C)(C)OC1CCC2(C)C(CCC3C2CCC2(C)C(C(C)CCCC(C)(C)O[Si](C)(C)CC)CCC3
Mol. weight [g/mol]: 577.08

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.62		Crippen Method
logp	11.082		Crippen Method
rinpol	3652.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R280029&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/66-782-1/5-alpha-cholestan-3-beta-25-diol-DMESI.pdf>

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