

(24S)-24-ethyl-5«alpha»-cholestan-3«beta»,24-diol

DMESI

InchiKey:

InChI=1S/C37H72O2Si2/c1-13-37(27(4)5,39-41(11,12)15-3)25-20-28(6)32-18-19-33-31-

SPGUWDQUZUDGSA-LVGRTLLHSA-N

Formula:

C37H72O2Si2

SMILES:

CCC(CCC(C)C1CCC2C3CCC4CC(O[Si](C)(C)CC)CCC4(C)C3CCC12C)(O[Si](C)(C)CC)

Mol. weight [g/mol]:

605.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.21		Crippen Method
logp	11.718		Crippen Method
rinpol	3690.00		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R279702&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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<https://www.cheméo.com/cid/67-520-0/24S-24-ethyl-5-alpha-cholestan-3-beta-24-diol-DMESI.pdf>

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