

5«alpha»-cholestan-3«beta»-ol (dihydrocholesterol), DMESI

Inchi: InChI=1S/C31H58OSi/c1-9-33(7,8)32-25-17-19-30(5)24(21-25)13-14-26-28-16-15-27(23)
InchiKey: NVSVPVNMQQAXHF-WFZDMNBNSA-N
Formula: C31H58OSi
SMILES: CC[Si](C)(C)OC1CCC2(C)C(CCC3C2CCC2(C)C(C(C)CCCC(C)C)CCC32)C1
Mol. weight [g/mol]: 474.88

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.45		Crippen Method
logp	9.718		Crippen Method
rinpol	3294.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R280049&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/61-433-3/5-alpha-cholestan-3-beta-ol-dihydrocholesterol-DMESI.pdf>

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