

24-Nor-3«alpha»,7«alpha»-dihydroxy-5«beta»-cholanoic acid, MeTMS

Inchi: C=1S/C30H56O4Si2/c1-20(17-27(31)32-4)23-11-12-24-28-25(14-16-30(23,24)3)29(2)
InchiKey: HCYJJSCVAJQMOY-CANWCQFHSA-N
Formula: C₃₀H₅₆O₄Si₂
SMILES: COC(=O)CC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 536.93

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.39		Crippen Method
logp	7.895		Crippen Method
rinpol	3119.00		NIST Webbook
rinpol	3119.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R271268&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/47-494-2/24-Nor-3-alpha-7-alpha-dihydroxy-5-beta-cholanoic-acid-MeTMS.pdf>

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