

4-Cholenoic acid, 7-«beta»-ol-3-one, TMS

Inchi: InChI=1S/C36H68O5Si4/c1-25(16-19-33(37)41-45(13,14)15)28-17-18-29-34-30(24-32(36)35)31-26-27-22-23-24
InchiKey: GLKHZJHSPOOTGF-KBEPPLKSA-N
Formula: C36H68O5Si4
SMILES: CC(CCC(=O)O[Si](C)(C)C)C1CCC2C3C(O[Si](C)(C)C)CC4=CC(O[Si](C)(C)C)=CCC4(C)C
Mol. weight [g/mol]: 693.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.53		Crippen Method
logp	10.365		Crippen Method
rinpol	3421.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R177389&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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