

7«alpha»,12«alpha»-dihydroxy-3-oxy-4-chol-24-oate-TMS

TMS

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C36H68O5Si4/c1-25(16-19-33(37)41-45(13,14)15)28-17-18-29-34-30(24-32(36)35)42-43-44-46-47-48-49-50-51-52-53-54-55-56-57-58-59-60-61-62-63-64-65-66-67-68/s1-36/t37,41,45,51,55,59,63,67

GLKHZJHSPOOTGF-RRSXFYFVSA-N

C36H68O5Si4

CC(CCC(=O)O[Si](C)(C)C)C1CCC2C3C(O[Si](C)(C)C)CC4=CC(O[Si](C)(C)C)=CCC4(C)C

693.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.53		Crippen Method
logp	10.365		Crippen Method
rinpol	3360.00		NIST Webbook
rinpol	3360.00		NIST Webbook

Sources

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R492574&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/24-117-5/7-alpha-12-alpha-dihydroxy-3-oxy-4-chol-24-oate-TMS.pdf>

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