

7«alpha»,12«alpha»,26-trihydroxy-4-cholesten-3-one-TMS

TMS

InchiKey:

InChI=1S/C39H76O4Si4/c1-28(27-40-44(5,6)7)18-17-19-29(2)32-20-21-33-37-34(26-36)(

ANQNBIFORCYFDW-APRKURMHSA-N

Formula:

C39H76O4Si4

SMILES:

CC(CCCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4=CC(O[Si](C)(C)C)=CCC4(C)C3CC(O[Si](C)(C)C)C1

Mol. weight [g/mol]:

721.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.77		Crippen Method
logp	11.865		Crippen Method
rinpol	3610.00		NIST Webbook
rinpol	3610.00		NIST Webbook

Sources

Crippen Method:

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

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R493953&Units=SI>

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/24-022-0/7-alpha-12-alpha-26-trihydroxy-4-cholesten-3-one-TMS.pdf>

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