

5«beta»-Cholane-3«alpha»,7«alpha»,12«alpha»,24

TMS

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C36H74O4Si4/c1-26(17-16-22-37-41(4,5)6)29-18-19-30-34-31(25-33(36(29,30

SQXKEDIKDUJREO-SSNUQJRFSA-N

C36H74O4Si4

CC(CCCO[Si](C)(C)C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CC

683.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.43		Crippen Method
logp	10.793		Crippen Method
rinpol	3278.00		NIST Webbook
rinpol	3278.00		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=R271639&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/31-660-4/5-beta-Cholane-3-alpha-7-alpha-12-alpha-24-tetrol-TMS.pdf>

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