

5«beta»-Cholestane-3«alpha»,7«alpha»,25-triol,

TMS

InchiKey:

InChI=1S/C35H70O3Si3/c1-25(17-20-33(2,3)38-41(12,13)14)28-15-16-29-32-30(19-22-3

TVNVZHJBEWPTJT-ONSBAMBLSA-N

Formula:

C35H70O3Si3

SMILES:

CC(CCC(C)(C)O[Si](C)(C)C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)

Mol. weight [g/mol]:

623.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.87		Crippen Method
logp	10.742		Crippen Method
rinpol	3462.00		NIST Webbook

Sources

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R271728&Units=SI>

Crippen Method:

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

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/65-032-4/5-beta-Cholestane-3-alpha-7-alpha-25-triol-TMS.pdf>

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