

5«beta»-Cholestane-3«alpha»,7«alpha»,24S,25-tetrol-TMS

TMS

InchiKey:

InChI=1S/C38H78O4Si4/c1-27(24-34(41-45(12,13)14)36(2,3)42-46(15,16)17)30-18-19-3

YDOXKJICRURTAJ-LJFVFAHASA-N

Formula:

C38H78O4Si4

SMILES:

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

Mol. weight [g/mol]:

711.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.37		Crippen Method
logp	11.572		Crippen Method
rinpol	3635.00		NIST Webbook

Sources

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R271713&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/30-167-3/5-beta-Cholestane-3-alpha-7-alpha-24S-25-tetrol-TMS.pdf>

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