

5«beta»-Homocholane-3«alpha»,7«alpha»,25-triol-TMS

TMS

InchiKey:

InChI=1S/C34H68O3Si3/c1-25(15-13-14-22-35-38(4,5)6)28-16-17-29-32-30(19-21-34(28

AUHPOWAMYQLWCU-KTRNCBEHSA-N

Formula:

C34H68O3Si3

SMILES:

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

Mol. weight [g/mol]:

609.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.34		Crippen Method
logp	10.353		Crippen Method
rinpol	3405.00		NIST Webbook

Sources

Crippen Method:

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

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R271768&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.cheméo.com/cid/16-756-5/5-beta-Homocholane-3-alpha-7-alpha-25-triol-TMS.pdf>

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