

5«beta»-Homocholane-3«alpha»,7«alpha»,12«alpha»-TMS

TMS

InchiKey:

InChI=1S/C37H76O4Si4/c1-27(18-16-17-23-38-42(4,5)6)30-19-20-31-35-32(26-34(37(30

XCJMPPVSTROYKS-RLIJUXHNSA-N

Formula:

C37H76O4Si4

SMILES:

CC(CCCCO[Si](C)(C)C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3C

Mol. weight [g/mol]:

697.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.84		Crippen Method
logp	11.183		Crippen Method
rinpol	3385.00		NIST Webbook
rinpol	3385.00		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R271753&Units=SI>

Crippen Method:

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

Crippen Method:

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

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/50-517-2/5-beta-Homocholane-3-alpha-7-alpha-12-alpha-25-tetrol-TMS.pdf>

Generated by Cheméo on 2024-04-25 20:27:46.039399818 +0000 UTC m=+16366114.959977130.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.