

2«alpha»,3«alpha»-cyclopropane-5«alpha»-andro

bisTMTBS
InChI=1S/C36H64O2Si2/c1-33(2,3)39(19-9-10-20-39)37-31-16-15-28-26-13-14-30-32(38)
InChIKey: QZBRKVKFHTWGNV-ZWEIHEGSSA-N

Formula:

C36H64O2Si2

SMILES:

CC12CCC3C(CCC4C(O[Si]5(C(C)(C)C)CCCC5)C5CC5CC34C)C1CCC2O[Si]1(C(C)(C)C)C

Mol. weight [g/mol]:

585.06

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.72		Crippen Method
logp	10.734		Crippen Method
rinpol	3930.00		NIST Webbook
rinpol	3930.00		NIST Webbook

Sources

Crippen Method:

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

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R385852&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/34-680-9/2-alpha-3-alpha-cyclopropane-5-alpha-androstan-4-alpha-17-beta-diol-bisTM>

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