

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

monoTMS
InChI: InChI=1S/C23H38O2Si/c1-22-11-10-18-15(17(22)8-9-20(22)24)6-7-19-21(25-26(3,4)5)16
InChIKey: XJQRLGLUGUAZNF-REKAFVNBSA-N

Formula:

C23H38O2Si

SMILES:

CC12CCC3C(CCC4C(O[Si](C)(C)C)C5CC5CC34C)C1CCC2=O

Mol. weight [g/mol]:

374.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.52		Crippen Method
logp	5.674		Crippen Method
rinpol	2630.00		NIST Webbook

Sources

Crippen Method:

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

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R385778&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.chemeo.com/cid/14-894-4/2-alpha-3-alpha-cyclopropane-5-alpha-androstan-17keto-4-alpha-ol-monoTMS>

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