

3«alpha»-Hydroxy-5«alpha»-pregnan-20-one, O-trimethylsilyl

Other names:

3«alpha»-Hydroxy-5«alpha»-pregnan-20-one-TMS
3-[(Trimethylsilyl)oxy]pregnan-20-one, (3«alpha»,5«alpha»)-
5-«alpha»-Pregnan-3-«alpha»-ol-20-one, TMS
5«alpha»-Pregnan-20-one, 3«alpha»-(trimethylsiloxy)-
5«ALPHA»-pregnan-3«alpha»-ol-20-one, tms derivative

Inchi:

InChI=1S/C24H42O2Si/c1-16(25)20-9-10-21-19-8-7-17-15-18(26-27(4,5)6)11-13-23(17,2

InchiKey:

GKHMQSZBQGVKC-OEMCAECPSA-N

Formula:

C24H42O2Si

SMILES:

CC(=O)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C

Mol. weight [g/mol]:

390.67

CAS:

18880-80-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.29		Crippen Method
logp	6.454		Crippen Method
rinpol	2622.00		NIST Webbook
rinpol	2622.00		NIST Webbook
rinpol	2622.00		NIST Webbook

Sources

Crippen Method:

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

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C18880803&Units=SI>

Legend

log10ws:

Log10 of Water solubility in mol/l

logp:

Octanol/Water partition coefficient

rinpol:

Non-polar retention indices

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