11«alpha»-Hydroxyprogesterone, trimethylsilyl ether

Other names: (11«alpha»)-11-[(Trimethylsilyl)oxy]pregn-4-ene-3,20-dione
11«ALPHA»-hydroxyprogesterone, tms derivative

Inchi: InChI=1S/C24H38O3Si/c1-15(25)19-9-10-20-18-8-7-16-13-17(26)11-12-23(16,2)22(18)2

InchiKey: WBASQZHRPPCPFM-UHFFFAOYSA-N

Formula: C24H38O3Si

SMILES: CC(=O)C1CCC2C3CCC4=CC(=O)CCC4(C)C3C(O[Si](C)(C)C)CC12C

Mol. weight [g/mol]: 402.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.66		Crippen Method
logp	5.553		Crippen Method
rinpol	3116.90		NIST Webbook
rinpol	3116.90		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U332963&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices