

# 3«beta»,5«beta»-Tetrahydrodeoxycorticosterone,

## MO-TMS

InchiKey:

InChI=1S/C28H53NO3Si2/c1-27-16-14-21(32-34(7,8)9)18-20(27)10-11-22-23-12-13-25(2

Formula:

C28H53NO3Si2

SMILES:

CON=C(CO[Si](C)(C)C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C

Mol. weight [g/mol]:

507.90

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.06		Crippen Method
logp	7.719		Crippen Method
rinpol	2924.00		NIST Webbook

## Sources

Crippen Method:

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

Crippen Method:

[https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R422045&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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