

3«beta»,5«alpha»-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	3045.00		NIST Webbook
rinpol	3045.00		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R422025&Units=SI>

Crippen Method:

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

Crippen Method:

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

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/21-231-1/3-beta-5-alpha-Tetrahydrodeoxycorticosterone-MO-TMS.pdf>

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