

3«alpha»,5«beta»-Tetrahydrodeoxycorticosterone

Other names:
MO-TMS

5«beta»-Pregnane-3«alpha», 21-diol-20-one, MO TMS

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

InchiKey: XPDALQOLOZEWHW-OHCZDJKISA-N

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
rinpola	2907.00		NIST Webbook
rinpola	2894.00		NIST Webbook
rinpola	2907.00		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=R421993&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpola: Non-polar retention indices

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