3«beta»,5«alpha»-Tetrahydrodeoxycorticosterone 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-HCAXFLNSSA-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
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/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