

11-Deoxycorticosterone, MO-TMS

Inchi: InChI=1S/C26H44N2O3Si/c1-25-14-12-19(27-29-3)16-18(25)8-9-20-21-10-11-23(26(21,22)17)24
InchiKey: QDEFZWVWFGZSRJ-RFSPMFOISA-N
Formula: C26H44N2O3Si
SMILES: CON=C1C=C2CCC3C(CCC4(C)C(C(CO[Si](C)(C)C)=NOC)CCC34)C2(C)CC1
Mol. weight [g/mol]: 460.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.31		Crippen Method
logp	6.422		Crippen Method
rinpol	3098.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R421864&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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