

11-Dehydrocorticosterone, MO-TMS

Inchi: InChI=1S/C26H42N2O4Si/c1-25-13-12-18(27-30-3)14-17(25)8-9-19-20-10-11-21(26(20,21)15)22-23-24-26
InchiKey: XVEOLMCMZXMYMLB-ZBLCBYOGSA-N
Formula: C₂₆H₄₂N₂O₄Si
SMILES: CON=C1C=C2CCC3C(C(=O)CC4(C)C(C(CO[Si](C)(C)C)=NOC)CCC34)C2(C)CC1
Mol. weight [g/mol]: 474.71

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.59		Crippen Method
logp	5.601		Crippen Method
rinpol	3196.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R421859&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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<https://www.cheméo.com/cid/67-801-8/11-Dehydrocorticosterone-MO-TMS.pdf>

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