

21-Hydroxyprogesterone, tert-butyldimethylsilyl ether

Other names: 21-Hydroxyprogesterone, tbdms derivative
Inchi: InChI=1S/C27H44O3Si/c1-25(2,3)31(6,7)30-17-24(29)23-11-10-21-20-9-8-18-16-19(28)1
InchiKey: XFKHARHPUCVJDK-UHFFFAOYSA-N
Formula: C₂₇H₄₄O₃Si
SMILES: CC12CCC(=O)C=C1CCC1C2CCC2(C)C(C(=O)CO[Si](C)(C)C(C)(C)C)CCC12
Mol. weight [g/mol]: 444.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.81		Crippen Method
logp	6.725		Crippen Method
rinpol	3403.30		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U333763&Units=SI>

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.chemeo.com/cid/86-356-2/21-Hydroxyprogesterone-tert-butyldimethylsilyl-ether.pdf>

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