

11«alpha»-Hydroxyprogesterone, TMS

Inchi: InChI=1S/C27H46O3Si2/c1-18(28)22-12-13-23-21-11-10-19-16-20(29-31(4,5)6)14-15-26
InchiKey: GGEFWIQQKCNVDB-QKSLXFNC-SA-N
Formula: C₂₇H₄₆O₃Si₂
SMILES: CC(=O)C1CCC2C3CCC4=CC(O[Si](C)(C)C)=CCC4(C)C3C(O[Si](C)(C)C)CC12C
Mol. weight [g/mol]: 474.82

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.12		Crippen Method
logp	7.330		Crippen Method
rinpol	2710.00		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=R305123&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/59-366-1/11-alpha-Hydroxyprogesterone-TMS.pdf>

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