

Pregnan-3,20,21-triol, TMS

Inchi: InChI=1S/C30H58O3Si3/c1-29-18-16-23(32-35(6,7)8)20-22(29)12-13-24-25-14-15-27(30)
InchiKey: RBSXFFWTNZTHKA-RWHPYDSTSA-N
Formula: C30H58O3Si3
SMILES: CC12CCC(O[Si](C)(C)C)CC1=CCC1C2CCC2(C)C(C(CO[Si](C)(C)C)O[Si](C)(C)C)CCC1
Mol. weight [g/mol]: 551.04

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.00		Crippen Method
logp	8.857		Crippen Method
rinpol	2999.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R394460&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/20-041-3/Pregnan-3-20-21-triol-TMS.pdf>

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