

Pregnan-1,3,16-triol-20-one, MeTMS

Inchi: InChI=1S/C30H58O4Si3/c1-20(31)28-26(33-36(7,8)9)19-25-23-14-13-21-17-22(32-35(4,5)6)30
InchiKey: TWRBBKDOJSRDLF-AACDYVSXSA-N
Formula: C30H58O4Si3
SMILES: CC(=O)C1C(O[Si](C)(C)C)CC2C3CCC4CC(O[Si](C)(C)C)CC(O[Si](C)(C)C)C4(C)C3CCO
Mol. weight [g/mol]: 567.04

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.30		Crippen Method
logp	8.114		Crippen Method
rinpol	2955.00		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=R393596&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/20-369-0/Pregnan-1-3-16-triol-20-one-MeTMS.pdf>

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