

Pregnan-1,3,16-triol, TMS

Inchi: InChI=1S/C30H58O3Si3/c1-13-24-27(32-35(7,8)9)20-26-23-15-14-21-18-22(31-34(4,5)6)
InchiKey: RNHJMXCYHINPLG-MQVJPIIYSA-N
Formula: C30H58O3Si3
SMILES: CCC1C(O[Si](C)(C)C)CC2C3CC=C4CC(O[Si](C)(C)C)CC(O[Si](C)(C)C)C4(C)C3CCC12
Mol. weight [g/mol]: 551.04

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.11		Crippen Method
logp	8.856		Crippen Method
rinpol	2955.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R394400&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/51-593-7/Pregnan-1-3-16-triol-TMS.pdf>

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