

5-Pregnen-2,3,20-triol, TMS

Inchi: InChI=1S/C30H58O3Si3/c1-21(31-34(4,5)6)24-15-16-25-23-14-13-22-19-27(32-35(7,8)9)
InchiKey: MAFMGPAYVBVTIC-JKOWSBFISA-N
Formula: C30H58O3Si3
SMILES: CC(O[Si](C)(C)C)C1CCC2C3CC=C4CC(O[Si](C)(C)C)C(O[Si](C)(C)C)CC4(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
rinsol	3068.00		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=R394217&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinsol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/55-047-9/5-Pregnen-2-3-20-triol-TMS.pdf>

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