

5«beta»-Pregnane-3«alpha»,16«alpha»,20«alpha»

EO-TMS

InChI=1S/C29H58O3Si3/c1-20(30-33(3,4)5)28-27(32-35(9,10)11)19-26-25-14-12-21-18-7
InChIKey: XTIFXEJHFJUBLK-VMQBTNLOSA-N
Formula: C29H58O3Si3
SMILES: CC(O[Si](C)(C)C)C1C(O[Si](C)(C)C)CC2C3CCC4CC(O[Si](C)(C)C)CCC4C3CCC21C
Mol. weight [g/mol]: 539.03

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.60		Crippen Method
logp	8.545		Crippen Method
rinpol	2871.00		NIST Webbook
rinpol	2872.00		NIST Webbook
rinpol	2871.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R527185&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/59-355-3/5-beta-Pregnane-3-alpha-16-alpha-20-alpha-triol-EO-TMS.pdf>

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