

5-«beta»-Pregnane-3«beta», 16«alpha», 20«alpha»-triol, MO TMS

Other names: 5«beta»-Pregnane-3«alpha», 16«alpha», 20«alpha»-triol, MO-TMS
Inchi: InChI=1S/C30H60O3Si3/c1-21(31-34(4,5)6)28-27(33-36(10,11)12)20-26-24-14-13-22-19
InchiKey: GKSDWCMXICLASA-MGXRMYDBSA-N
Formula: C30H60O3Si3
SMILES: CC(O[Si](C)(C)C)C1C(O[Si](C)(C)C)CC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC21O
Mol. weight [g/mol]: 553.05

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.02		Crippen Method
logp	8.935		Crippen Method
rinpol	2906.00		NIST Webbook
rinpol	2894.00		NIST Webbook
rinpol	2872.00		NIST Webbook
rinpol	2872.00		NIST Webbook

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=R250469&Units=SI>

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/37-022-6/5-beta-Pregnane-3-beta-16-alpha-20-alpha-triol-MO-TMS.pdf>

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