

Pregnan-2,3,20-triol, TMS

Other names: Pregnane-2,3,20-triol, TMS
Inchi: InChI=1S/C30H60O3Si3/c1-21(31-34(4,5)6)24-15-16-25-23-14-13-22-19-27(32-35(7,8)9)
InchiKey: KXOPUEFDTRWMJL-UHFFFAOYSA-N
Formula: C30H60O3Si3
SMILES: CC(O[Si](C)(C)C)C1CCC2C3CCC4CC(O[Si](C)(C)C)C(O[Si](C)(C)C)CC4(C)C3CCC12C
Mol. weight [g/mol]: 553.05

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.02		Crippen Method
logp	8.935		Crippen Method
rinpol	2899.00		NIST Webbook
rinpol	2935.00		NIST Webbook
rinpol	2949.00		NIST Webbook
rinpol	2899.00		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=R265986&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/57-624-6/Pregnan-2-3-20-triol-TMS.pdf>

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