

16«alpha»-Methylpregnenolone, TMS

Inchi: InChI=1S/C25H42O2Si/c1-16-14-22-20-9-8-18-15-19(27-28(5,6)7)10-12-24(18,3)21(20)1
InchiKey: JOYGRUHLOYRWGM-BXWWMJJPSA-N
Formula: C25H42O2Si
SMILES: CC(=O)C1C(C)CC2C3CC=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC21C
Mol. weight [g/mol]: 402.69

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.56		Crippen Method
logp	6.621		Crippen Method
rinpol	2714.00		NIST Webbook
rinpol	2714.00		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=R305143&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/62-972-4/16-alpha-Methylpregnenolone-TMS.pdf>

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