

5«beta»-Pregnane-3«beta»-ol-20-one, MO TMS

Inchi: InChI=1S/C25H45NO2Si/c1-17(26-27-4)21-10-11-22-20-9-8-18-16-19(28-29(5,6)7)12-14
InchiKey: MFOIVZWKNBPHHX-FRBWRTIZSA-N
Formula: C25H45NO2Si
SMILES: CON=C(C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 419.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.67		Crippen Method
logp	6.888		Crippen Method
rinpol	2737.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R250543&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/42-635-0/5-beta-Pregnane-3-beta-ol-20-one-MO-TMS.pdf>

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