

5-«alpha»-Pregnan-20-«alpha»-ol-11-one, MO-TMS

Inchi: InChI=1S/C25H45NO2Si/c1-17(28-29(5,6)7)20-13-14-21-19-12-11-18-10-8-9-15-24(18,2)
InchiKey: AENBXJWUEFXGGT-GLQYAXMESA-N
Formula: C25H45NO2Si
SMILES: CON=C1CC2(C)C(C(C)O[Si](C)(C)C)CCC2C2CCC3CCCCC3(C)C12
Mol. weight [g/mol]: 419.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.67		Crippen Method
logp	6.888		Crippen Method
rinpol	2670.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R486430&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/32-127-5/5-alpha-Pregnan-20-alpha-ol-11-one-MO-TMS.pdf>

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