

5-«beta»-Pregnan-3-one-11-«beta»-ol, MO-TMS

Inchi: InChI=1S/C25H45NO2Si/c1-8-17-10-12-21-20-11-9-18-15-19(26-27-4)13-14-24(18,2)23
InchiKey: FOLJPVIGGPQYMO-NXOAMMRSSA-N
Formula: C25H45NO2Si
SMILES: CCC1CCC2C3CCC4CC(=NOC)CCC4(C)C3C(O[Si](C)(C)C)CC12C
Mol. weight [g/mol]: 419.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.67		Crippen Method
logp	6.888		Crippen Method
rinpol	2621.00		NIST Webbook
rinpol	2679.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R486123&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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/44-035-4/5-beta-Pregnan-3-one-11-beta-ol-MO-TMS.pdf>

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