

5-«beta»-Pregnan-20-«beta»-ol, TMS

Inchi: InChI=1S/C24H44OSi/c1-17(25-26(4,5)6)20-12-13-21-19-11-10-18-9-7-8-15-23(18,2)22(19,20)21
InchiKey: RGJNVEQQKVLRFZ-MBEPHZASSA-N
Formula: C24H44OSi
SMILES: CC(O[Si](C)(C)C)C1CCC2C3CCC4CCCCC4(C)C3CCC12C
Mol. weight [g/mol]: 376.69

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.01		Crippen Method
logp	7.275		Crippen Method
rinpol	2463.00		NIST Webbook
rinpol	2463.00		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=R486896&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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<https://www.chemeo.com/cid/63-885-0/5-beta-Pregnan-20-beta-ol-TMS.pdf>

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