

5-«beta»-Pregnan-3-«beta»-ol, TMS

Inchi: InChI=1S/C24H44OSi/c1-7-17-9-11-21-20-10-8-18-16-19(25-26(4,5)6)12-14-24(18,3)22(23)H
InchiKey: QMRHJLFVINTSBH-JRXGDUPLSA-N
Formula: C₂₄H₄₄OSi
SMILES: CCC1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(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	2402.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R487131&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/35-696-1/5-beta-Pregnan-3-beta-ol-TMS.pdf>

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