

5-«beta»-Pregnan-3-«alpha»,20-«beta»-diol, TMS

Inchi: InChI=1S/C27H52O2Si2/c1-19(28-30(4,5)6)23-12-13-24-22-11-10-20-18-21(29-31(7,8)9)
InchiKey: PSZRAFDARWUCMW-WPBWPDMKSA-N
Formula: C27H52O2Si2
SMILES: CC(O[Si](C)(C)C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 464.87

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.51		Crippen Method
logp	8.105		Crippen Method
rinpol	2749.00		NIST Webbook
rinpol	2772.00		NIST Webbook
rinpol	2743.00		NIST Webbook
rinpol	2768.00		NIST Webbook
rinpol	2767.00		NIST Webbook
rinpol	2749.00		NIST Webbook
rinpol	2766.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R385189&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/35-685-3/5-beta-Pregnan-3-alpha-20-beta-diol-TMS.pdf>

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