

5-«beta»-Pregnan-3-«beta»,20-«alpha»-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-JOPQZIHYS-A-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	2780.00		NIST Webbook
rinpol	2750.00		NIST Webbook
rinpol	2782.00		NIST Webbook
rinpol	2750.00		NIST Webbook
rinpol	2757.00		NIST Webbook
rinpol	2757.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R384502&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/35-280-2/5-beta-Pregnan-3-beta-20-alpha-diol-TMS.pdf>

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