

5-«alpha»-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-SXFMRIJJSA-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	2746.00		NIST Webbook
rinpol	2767.00		NIST Webbook
rinpol	2758.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R384988&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.cheméo.com/cid/52-400-9/5-alpha-Pregnan-3-alpha-20-beta-diol-TMS.pdf>

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